

1. BTE

CAS Registry Number: 556809-76-8

C₂₅ H₁₈ F₆ S₄

2,2'-Bithiophene, 4-[2-(5,5'-dimethyl[2,2'-bithiophen]-4-yl)-3,3,4,4,5,5-hexafluoro-1-cyclopenten-1-yl]-5,5'-dimethyl-

2,2'-Bithiophene, 4,4''-(3,3,4,4,5,5-hexafluoro-1-cyclopentene-1,2-diyl)bis[5,5'-dimethyl-(9CI)]

Source of Registration: CA

[~5 References](#)

Document Types:

Journal,

Patent

CAplus Role	Patents	Nonpatents
Preparation	✓	✓
Process		✓
Properties		✓
Reactant or reagent		✓
Uses	✓	✓

Predicted Properties: [Biological](#) [Chemical](#) [Density](#) [Lipinski and Related Spectra](#) [Structure-related](#) [Thermal](#)

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Biological Properties	Value	Conditions	Notes
Bioconcentration Factor	1.00E6	pH 1 Temp: 25 °C	(4)
Bioconcentration Factor	1.00E6	pH 2 Temp: 25 °C	(4)
Bioconcentration Factor	1.00E6	pH 3 Temp: 25 °C	(4)
Bioconcentration Factor	1.00E6	pH 4 Temp: 25 °C	(4)
Bioconcentration Factor	1.00E6	pH 5 Temp: 25 °C	(4)
Bioconcentration Factor	1.00E6	pH 6 Temp: 25 °C	(4)
Bioconcentration Factor	1.00E6	pH 7 Temp: 25 °C	(4)
Bioconcentration Factor	1.00E6	pH 8 Temp: 25 °C	(4)
Bioconcentration Factor	1.00E6	pH 9 Temp: 25 °C	(4)
Bioconcentration Factor	1.00E6	pH 10 Temp: 25 °C	(4)

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Chemical Properties	Value	Conditions	Notes
Koc	5.01E6	pH 1 Temp: 25 °C	(4)
Koc	5.01E6	pH 2 Temp: 25 °C	(4)
Koc	5.01E6	pH 3 Temp: 25 °C	(4)

Koc	5.01E6	pH 4 Temp: 25 °C	(4)
Koc	5.01E6	pH 5 Temp: 25 °C	(4)
Koc	5.01E6	pH 6 Temp: 25 °C	(4)
Koc	5.01E6	pH 7 Temp: 25 °C	(4)
Koc	5.01E6	pH 8 Temp: 25 °C	(4)
Koc	5.01E6	pH 9 Temp: 25 °C	(4)
Koc	5.01E6	pH 10 Temp: 25 °C	(4)
logD	9.78	pH 1 Temp: 25 °C	(4)
logD	9.78	pH 2 Temp: 25 °C	(4)
logD	9.78	pH 3 Temp: 25 °C	(4)
logD	9.78	pH 4 Temp: 25 °C	(4)
logD	9.78	pH 5 Temp: 25 °C	(4)
logD	9.78	pH 6 Temp: 25 °C	(4)
logD	9.78	pH 7 Temp: 25 °C	(4)
logD	9.78	pH 8 Temp: 25 °C	(4)
logD	9.78	pH 9 Temp: 25 °C	(4)
logD	9.78	pH 10 Temp: 25 °C	(4)
logP	9.784±0.965	Temp: 25 °C	(4)
Mass Intrinsic Solubility	Sparingly Soluble (1.6E-7 g/L) Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 1 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 2 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 3 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 4 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 5 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 6 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 7 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 8 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 9 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) pH 10 Temp: 25 °C		(4)
Mass Solubility	Sparingly Soluble (1.6E-7 g/L) Unbuffered Water pH 7.00 Temp: 25 °C		(4)
Molar Intrinsic Solubility	Sparingly Soluble (2.8E-10 mol/L) Temp: 25 °C		(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L) pH 1 Temp: 25 °C		(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L) pH 2 Temp: 25 °C		(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L) pH 3 Temp: 25 °C		(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L) pH 4 Temp: 25 °C		(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L) pH 5 Temp: 25 °C		(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L) pH 6 Temp: 25 °C		(4)

Molar Solubility	Sparingly Soluble (2.8E-10 mol/L)	pH 7 Temp: 25 °C	(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L)	pH 8 Temp: 25 °C	(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L)	pH 9 Temp: 25 °C	(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L)	pH 10 Temp: 25 °C	(4)
Molar Solubility	Sparingly Soluble (2.8E-10 mol/L)	Unbuffered Water pH 7.00 Temp: 25 °C	(4)
Molecular Weight	560.66		(4)
Vapor Pressure	2.90E-11 Torr	Temp: 25 °C	(4)

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Density Properties	Value	Conditions	Notes
Density	1.48±0.1 g/cm ³	Temp: 20 °C Press: 760 Torr	(4)
Molar Volume	378.5±5.0 cm ³ /mol	Temp: 20 °C Press: 760 Torr	(4)

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Lipinski and Related Properties	Value	Conditions	Notes
Freely Rotatable Bonds	4		(4)
H Acceptors	0		(4)
H Donors	0		(4)
H Donor/Acceptor Sum	0		(4)
logP	9.784±0.965	Temp: 25 °C	(4)
Molecular Weight	560.66		(4)

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Spectra Properties	Value	Conditions	Notes
Carbon-13 NMR Spectrum	See spectrum		(5)
Proton NMR Spectrum	See spectrum		(5)

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Structure-related Properties	Value	Conditions	Notes
Polar Surface Area	113 A ²		(4)

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Thermal Properties	Value	Conditions	Notes
Boiling Point	542.1±50.0 °C	Press: 760 Torr	(4)
Enthalpy of Vaporization	78.94±3.0 kJ/mol	Press: 760 Torr	(4)
Flash Point	281.6±30.1 °C		(4)

- (4) Calculated using Advanced Chemistry Development (ACD/Labs) Software V9.04 for Solaris (© 1994-2009 ACD/Labs)
- (5) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V9.07 (© 1994-2009 ACD/Labs)

Experimental Properties: [Chemical](#) [Electrical](#) [Spectra](#) [Thermal](#)

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Chemical Properties	Value	Conditions	Notes
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Potential of Electrode ReactionSee full text [\(1\)](#) CAS
Potential of Electrode ReactionSee full text [\(2\)](#) CAS

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Electrical Properties	Value	Conditions	Notes
Electric Current-Potential Curve	See full text		(1) CAS

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Spectra Properties	Value	Conditions	Notes
Carbon-13 NMR Spectrum	See full text		(1) CAS
Carbon-13 NMR Spectrum	See full text		(2) CAS
IR Absorption Spectrum	See full text		(2) CAS
Mass Spectrum	See full text		(2) CAS
Proton NMR Spectrum	See full text		(1) CAS
Proton NMR Spectrum	See full text		(2) CAS
UV and Visible Absorption Spectrum	See full text		(1) CAS
UV and Visible Spectrum	See full text		(3) CAS

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Thermal Properties	Value	Conditions	Notes
Melting Point	124-125 °C		(2) CAS
Melting Point	See full text		(1) CAS

- [\(1\) Peters, Andrea; Chemical Communications \(Cambridge, United Kingdom\) 2003, \(8\), P954-955 CAPLUS](#)
- [\(2\) Branda, Neil R.; WO 2004015024 A1 2004 CAPLUS](#)
- [\(3\) Andrew, Trisha L.; Science \(Washington, DC, United States\) 2009, V324\(5929\), P917-921 CAPLUS](#)

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