2,2'-Bithiophene

Other names:	2,2'-Dithienyl
	2,2'-Dithiophene
	2,2'-bithienyl
	Dithienyl
Inchi:	InChI=1S/C8H6S2/c1-3-7(9-5-1)8-4-2-6-10-8/h1-6H
InchiKey:	OHZAHWOAMVVGEL-UHFFFAOYSA-N
Formula:	C8H6S2
SMILES:	c1csc(-c2cccs2)c1
Mol. weight [g/mol]:	166.26
CAS:	492-97-7

Physical Properties

Property code	Value	Unit	Source
ea	0.07 ± 0.02	eV	NIST Webbook
ea	0.05 ± 0.01	eV	NIST Webbook
hfus	16.50	kJ/mol	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
hsub	85.20 ± 0.40	kJ/mol	NIST Webbook
ie	7.83	eV	NIST Webbook
log10ws	-3.59		Crippen Method
logp	3.477		Crippen Method
mcvol	117.360	ml/mol	McGowan Method
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
tb	533.20	K	NIST Webbook
tb	533.00	K	NIST Webbook
tf	306.00	K	NIST Webbook
tf	305.00 ± 4.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	16.50	kJ/mol	304.20	NIST Webbook

hsubt	86.00 ± 0.40	kJ/mol	283.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.70	K	1.60	NIST Webbook
tbrp	399.50 ± 1.50	K	1.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C492977&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives:	https://www.doi.org/10.1016/j.tca.2005.11.024
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ea:	Electron affinity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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