3,3'-Bithiophene

Other names:	3,3'-Dithienyl
	3,3'-bithienyl
Inchi:	InChI=1S/C8H6S2/c1-3-9-5-7(1)8-2-4-10-6-8/h1-6H
InchiKey:	IAAQEGBHNXAHBF-UHFFFAOYSA-N
Formula:	C8H6S2
SMILES:	c1cc(-c2ccsc2)cs1
Mol. weight [g/mol]:	166.26
CAS:	3172-56-3

Physical Properties

Property code	Value	Unit	Source
hsub	89.20 ± 0.30	kJ/mol	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	7.99	eV	NIST Webbook
ie	7.99	eV	NIST Webbook
log10ws	-3.59		Crippen Method
logp	3.477		Crippen Method
mcvol	117.360	ml/mol	McGowan Method
tf	406.20	K	Phase transition equilibrium of terthiophene isomers

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	88.60 ± 0.30	kJ/mol	309.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase transition equilibrium of terthiophene isomers:	https://www.doi.org/10.1016/j.jct.2010.08.007
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3172563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
tf:	Normal melting (fusion) point