Thieno[3,2-b]thiophene

Other names:	1,4-Dithiapentalene
	1,4-Thiophthene
Inchi:	InChI=1S/C6H4S2/c1-3-7-6-2-4-8-5(1)6/h1-4H
InchiKey:	VJYJJHQEVLEOFL-UHFFFAOYSA-N
Formula:	C6H4S2
SMILES:	c1cc2sccc2s1
Mol. weight [g/mol]:	140.23
CAS:	251-41-2

Physical Properties

Property code	Value	Unit	Source
ie	8.10	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.14	eV	NIST Webbook
log10ws	-2.79		Crippen Method
logp	2.963		Crippen Method
mcvol	93.480	ml/mol	McGowan Method
rinpol	1214.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	201.53		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1214.00		NIST Webbook
ripol	1843.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1872.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C251412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
ripol:	Polar retention indices