

Thieno[2,3-b]thiophene

Inchi: InChI=1S/C6H4S2/c1-3-7-6-5(1)2-4-8-6/h1-4H
InchiKey: YHBTXTFFTYXOFV-UHFFFAOYSA-N
Formula: C6H4S2
SMILES: c1cc2ccsc2s1
Mol. weight [g/mol]: 140.23
CAS: 250-84-0

Physical Properties

Property code	Value	Unit	Source
ie	8.45	eV	NIST Webbook
ie	8.32	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
ie	8.32	eV	NIST Webbook
log10ws	-2.79		Crippen Method
logp	2.963		Crippen Method
mvol	93.480	ml/mol	McGowan Method
rinpol	201.25		NIST Webbook
rinpol	201.25		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1212.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C250840&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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