2-(Methylmercapto)benzothiazole

Other names:	Benzothiazole, 2-(methylthio)- 2-(Methylthio)benzothiazole 2-(Methylthio)benzothiozole
Inchi:	InChI=1S/C8H7NS2/c1-10-8-9-6-4-2-3-5-7(6)11-8/h2-5H,1H3
InchiKey:	UTBVIMLZIRIFFR-UHFFFAOYSA-N
Formula:	C8H7NS2
SMILES:	CSc1nc2ccccc2s1
Mol. weight [g/mol]:	181.28
CAS:	615-22-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	3.018		Crippen Method
mcvol	127.340	ml/mol	McGowan Method
rinpol	272.73		NIST Webbook
rinpol	273.74		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	272.73		NIST Webbook
rinpol	1589.00		NIST Webbook
ripol	2422.00		NIST Webbook
ripol	2422.00		NIST Webbook
ripol	2422.00		NIST Webbook
ripol	2422.00		NIST Webbook
ripol	2422.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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