

2(3H)-Benzothiazolethione, 6-ethoxy-

Other names:	2-Mercapto-6-ethoxybenzothiazole 6-Ethoxy-2-mercaptobenzothiazole USAF pd-58 2-Benzothiazolethiol, 6-ethoxy-
Inchi:	InChI=1S/C9H9NOS2/c1-2-11-6-3-4-7-8(5-6)13-9(12)10-7/h3-5H,2H2,1H3,(H,10,12)
InchiKey:	HOASVNMVYBSLSU-UHFFFAOYSA-N
Formula:	C9H9NOS2
SMILES:	CCOc1ccc2nc(S)sc2c1
Mol. weight [g/mol]:	211.30
CAS:	120-53-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	2.984		Crippen Method
mcvol	147.300	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120536&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

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