

4-Morpholinecarbodithioic acid, 3-mercaptopropyl ester

Inchi:	InChI=1S/C8H15NOS3/c11-6-1-7-13-8(12)9-2-4-10-5-3-9/h11H,1-7H2
InchiKey:	FGWHCEACJXWVBS-UHFFFAOYSA-N
Formula:	C8H15NOS3
SMILES:	S=C(SCCCS)N1CCOCC1
Mol. weight [g/mol]:	237.41
CAS:	64226-32-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	1.657		Crippen Method
mcvol	173.320	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64226320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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