

N-Morpholinomethyl-isopropyl-sulfide

Other names:	1-Isopropylthiomethylmorpholine
Inchi:	InChI=1S/C8H17NOS/c1-8(2)11-7-9-3-5-10-6-4-9/h8H,3-7H2,1-2H3
InchiKey:	YXTBTNKSZYWAUTA-UHFFFAOYSA-N
Formula:	C8H17NOS
SMILES:	CC(C)SCN1CCOCC1
Mol. weight [g/mol]:	175.29
CAS:	77422-34-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.21		Crippen Method
logp	1.418		Crippen Method
mcvol	144.920	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77422345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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