

2-Morpholinoethyl isothiocyanate

Inchi:	InChI=1S/C7H12N2OS/c11-7-8-1-2-9-3-5-10-6-4-9/h1-6H2
InchiKey:	SDNSCXCVQHBGH-UHFFFAOYSA-N
Formula:	C7H12N2OS
SMILES:	S=C=NCCN1CCOCC1
Mol. weight [g/mol]:	172.25
CAS:	63224-35-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.24		Crippen Method
logp	0.421		Crippen Method
mcvol	132.210	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63224351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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