3-Morpholinopropyl isothiocyanate

Inchi:	InChI=1S/C8H14N2OS/c12-8-9-2-1-3-10-4-6-11-7-5-10/h1-7H2
InchiKey:	BCEFDMYFAAAFPE-UHFFFAOYSA-N
Formula:	C8H14N2OS
SMILES:	S=C=NCCCN1CCOCC1
Mol. weight [g/mol]:	186.28
CAS:	32813-50-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.66		Crippen Method
logp	0.812		Crippen Method
mcvol	146.300	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32813506&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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