

4-Morpholinepropanoic acid, methyl ester

Inchi:	InChI=1S/C8H15NO3/c1-11-8(10)2-3-9-4-6-12-7-5-9/h2-7H2,1H3
InchiKey:	YMSLLIGKMYXCPK-UHFFFAOYSA-N
Formula:	C8H15NO3
SMILES:	COC(=O)CCN1CCOCC1
Mol. weight [g/mol]:	173.21
CAS:	33611-43-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.41		Crippen Method
logp	-0.118		Crippen Method
mcvol	136.010	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=C33611437&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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