

Morpholine, 4,4'-malonyldi-

Inchi:	InChI=1S/C11H18N2O4/c14-10(12-1-5-16-6-2-12)9-11(15)13-3-7-17-8-4-13/h1-9H2
InchiKey:	DPNZFWSVHKTMAF-UHFFFAOYSA-N
Formula:	C11H18N2O4
SMILES:	O=C(CC(=O)N1CCOCC1)N1CCOCC1
Mol. weight [g/mol]:	242.27
CAS:	10256-01-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.92		Crippen Method
logp	-0.906		Crippen Method
mcvol	178.970	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=C10256016&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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<https://www.chemeo.com/cid/120-514-7/Morpholine-4-4-malonyldi.pdf>

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