

Dichloroacetic acid, morpholide

Inchi: InChI=1S/C6H9Cl2NO2/c7-5(8)6(10)9-1-3-11-4-2-9/h5H,1-4H2
InchiKey: SPDHGKQMFGYCHN-UHFFFAOYSA-N
Formula: C6H9Cl2NO2
SMILES: O=C(C(Cl)Cl)N1CCOCC1
Mol. weight [g/mol]: 198.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.57		Crippen Method
logp	0.649		Crippen Method
mcvol	126.440	ml/mol	McGowan Method
rinpole	1359.00		NIST Webbook

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=U307295&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/16-975-2/Dichloroacetic-acid-morpholide.pdf>

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