

Mercumallylic acid

Inchi: InChI=1S/C14H14O6/c1-19-10(7-15)5-8-3-2-4-9-6-11(13(16)17)14(18)20-12(8)9/h2-4,6,11-13,15-18,20
InchiKey: LNSCQJMHUICSSU-UHFFFAOYSA-N
Formula: C14H14O6
SMILES: COC(CO)Cc1cccc2cc(C(=O)O)c(=O)oc12
Mol. weight [g/mol]: 278.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.60		Crippen Method
logp	1.041		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
rinpol	2074.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R18058&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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/65-515-8/Mercumallylic-acid.pdf>

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