

Procerine

Inchi: InChI=1S/C13H21NO5/c1-7(8(2)16)13(18)19-11-3-4-14-5-10(17)9(6-15)12(11)14/h7,9-12
InchiKey: UEASBNMLRVSIIE-GCZKNKFQBSA-N
Formula: C13H21NO5
SMILES: CC(=O)C(C)C(=O)OC1CCN2CC(O)C(CO)C12
Mol. weight [g/mol]: 271.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.15		Crippen Method
logp	-0.819		Crippen Method
mcvol	203.040	ml/mol	McGowan Method
rinpol	1974.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R636630&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/83-231-3/Procerine.pdf>

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