

Pycnanthine

Inchi: InChI=1S/C20H31NO7/c1-12(2)20(26,14(4)23)19(25)27-11-15-5-7-21-8-6-16(18(15)21)2
InchiKey: UKPSUWZPUAENNH-LNEDORHWSA-N
Formula: C20H31NO7
SMILES: CC(=CC(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)C)C(C)O)C12)CO
Mol. weight [g/mol]: 397.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.98		Crippen Method
logp	0.162		Crippen Method
mcvol	304.810	ml/mol	McGowan Method
rinpola	2793.00		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=R299622&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/41-284-1/Pycnanthine.pdf>

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