

Parsonsine

Inchi: InChI=1S/C23H37NO7/c1-13(2)17-10-19(25)29-12-16-6-8-24-9-7-18(21(16)24)31-22(27)
InchiKey: IWRWQFWNXAFSBO-SMKAEANXSA-N
Formula: C23H37NO7
SMILES: CC(C)C1CC(=O)OCC2CCN3CCC(OC(=O)C(O)(C(C)C)CC(=O)OC1C)C23
Mol. weight [g/mol]: 439.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	1.920		Crippen Method
mcvol	340.520	ml/mol	McGowan Method
rinpola	2818.00		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=R178471&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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/44-434-1/Parsonsine.pdf>

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