

7-O-Acetylechinate

Inchi: InChI=1S/C17H27NO6/c1-10(2)17(22,11(3)19)16(21)23-9-13-5-7-18-8-6-14(15(13)18)24
InchiKey: RKDOFSJTBIDAHX-FIUQPQMISA-N
Formula: C17H27NO6
SMILES: CC(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)C)C(C)O)C12
Mol. weight [g/mol]: 341.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	0.244		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
rinpol	2235.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R299677&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/16-168-8/7-O-Acetylechinate.pdf>

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