

7-(2-Methylbutyryl)-9-(2,3-dihydroxybutyryl)retronecine

Inchi:	InChI=1S/C17H27NO6/c1-4-10(2)16(21)24-13-6-8-18-7-5-12(14(13)18)9-23-17(22)15(20)
InchiKey:	URBUCYRYSVLIOW-QIUSFHBQSA-N
Formula:	C17H27NO6
SMILES:	CCC(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)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	2285.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R299568&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

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