7-diacetylintermedine

Inchi: InChI=1S/C19H29NO8/c1-11(27-12(2)21)19(25,18(4,5)24)17(23)26-10-14-6-8-20-9-7-15
InchiKey: KULWDUGOUHVLGZ-JBQFIWDSSA-N
Formula: C19H29NO8
SMILES: CC(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)OC(C)=O)C(C)(C)O)C12
Mol. weight [g/mol]: 399.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	-0.071		Crippen Method
mcvol	296.590	ml/mol	McGowan Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R227880&Units=SI
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

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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