Retusamine

Inchi: InChI=1S/C19H25NO7/c1-5-19-11(2)18(3,27-17(19)24)15(22)25-10-12-6-8-20(4)9-7-13(1
InchiKey: DEVNDOKWQVKIND-MMTOQGCZSA-N
Formula: C19H25NO7
SMILES: CCC12C(=O)OC3CCN(C)CC=C(COC(=O)C(C)(OC1=O)C2C)C3=O
Mol. weight [g/mol]: 379.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	0.634		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R590346&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.