[(1R,8R)-7-(Hydroxymethyl)-2,3,5,8-tetrahydro-1H-
(E)-4-hydroxy-3-methyl-but-2-enoate

InChI: InChI=1S/C14H21NO4/c1-10(7-16)6-13(18)19-9-12-3-5-15-4-2-11(8-17)14(12)15/h2,6,12
InChIKey: MPQIEDCEYHDXGK-VABZHALQSA-N
Formula: C14H21NO4
SMILES: CC(=CC(=O)OCC1CCN2CC=C(CO)C12)CO
Mol. weight [g/mol]: 267.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	0.091		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R577803&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

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