3-(2'-Hydroxytropoyloxy)-6,7-epoxytropane

Inchi: InChI=1S/C17H21NO5/c1-18-12-7-11(8-13(18)15-14(12)23-15)22-16(20)17(21,9-19)10-5
InchiKey: JEJREKXHLFEVHN-MWJIJGFASA-N
Formula: C17H21NO5
SMILES: CN1C2CC(OC(=O)C(O)(CO)c3ccccc3)CC1C1OC12
Mol. weight [g/mol]: 319.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	0.022		Crippen Method
mcvol	229.080	ml/mol	McGowan Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		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=R421304&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.