Isomer of 1«beta»,2«beta»-Epoxy-1«alpha»-hydroxymethyl-

Inchi: InChI=1S/C8H13NO2/c10-5-8-6-2-1-3-9(6)4-7(8)11-8/h6-7,10H,1-5H2/t6?,7-,8+/m1/s1
InchiKey: FRPJEHRSJNAWEI-VVXQKDJTSA-N
Formula: C8H13NO2
SMILES: OCC12OC1CN1CCCC12
Mol. weight [g/mol]: 155.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.11		Crippen Method
logp	-0.406		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
rinpol	1360.00		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=R590306&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