

Scopoline

Inchi: InChI=1S/C8H13NO2/c1-9-5-2-4-3-6(9)8(11-4)7(5)10/h4-8,10H,2-3H2,1H3
InchiKey: MEGPURSNXMUDAE-UHFFFAOYSA-N
Formula: C8H13NO2
SMILES: CN1C2CC3CC1C(O3)C2O
Mol. weight [g/mol]: 155.19
CAS: 487-27-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.34		Crippen Method
logp	-0.409		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
rinpol	1230.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1230.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C487274&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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