

Senecicannabine

Inchi: InChI=1S/C18H23NO7/c1-10-18(26-10)8-17(9-24-17)16(2,22)14(20)23-7-11-3-5-19-6-4-
InchiKey: LTFQUYMOUGXPEW-QWEHXZQISA-N
Formula: C18H23NO7
SMILES: CC1OC12CC1(CO1)C(C)(O)C(=O)OCC1=CCN3CCC(OC2=O)C13
Mol. weight [g/mol]: 365.38
CAS: 81855-31-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Crippen Method
logp	-0.463		Crippen Method
mcvol	248.350	ml/mol	McGowan Method
rinpole	2618.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C81855314&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/40-605-5/Senecicannabine.pdf>

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