

Heliotrine (7S)

Inchi: InChI=1S/C16H27NO5/c1-10(2)16(20,11(3)21-4)15(19)22-9-12-5-7-17-8-6-13(18)14(12)
InchiKey: LMFKRLGHEKVMNT-ZGMNHVEMSA-N
Formula: C16H27NO5
SMILES: COC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)C
Mol. weight [g/mol]: 313.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	0.327		Crippen Method
mcvol	245.310	ml/mol	McGowan Method
rinpol	2100.00		NIST Webbook
rinpol	2114.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178228&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/10-226-9/Heliotrine-7S.pdf>

Generated by Cheméo on 2025-12-21 23:19:56.601769771 +0000 UTC m=+6107394.131810443.

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