

Indicine

Inchi:	InChI=1S/C15H25NO5/c1-9(2)15(20,10(3)17)14(19)21-8-11-4-6-16-7-5-12(18)13(11)16/
InchiKey:	SFVVQRJOGUKCEG-UOFHRTMOSA-N
Formula:	C15H25NO5
SMILES:	CC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)O
Mol. weight [g/mol]:	299.36
CAS:	480-82-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.17		Crippen Method
logp	-0.327		Crippen Method
mcvol	231.220	ml/mol	McGowan Method
rinpol	2126.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2126.00		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=C480820&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

Latest version available from:

<https://www.chemeo.com/cid/31-920-5/Indicine.pdf>

Generated by Cheméo on 2025-12-23 18:13:04.019966086 +0000 UTC m=+6261781.550006750.

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