

Isonipecotic acid, N-acryloyl-, tetradecyl ester

Inchi: InChI=1S/C23H41NO3/c1-3-5-6-7-8-9-10-11-12-13-14-15-20-27-23(26)21-16-18-24(19-1
InchiKey: MOFNWSLGLHJXEW-UHFFFAOYSA-N
Formula: C23H41NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCCCCCCCCCCCC)CC1
Mol. weight [g/mol]: 379.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.16		Crippen Method
logp	5.655		Crippen Method
mcvol	338.760	ml/mol	McGowan Method
rinpol	3034.00		NIST Webbook
rinpol	3034.00		NIST Webbook

Sources

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=U361063&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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