

Isonipecotic acid, N-acryloyl-, ethyl ester

Inchi: InChI=1S/C11H17NO3/c1-3-10(13)12-7-5-9(6-8-12)11(14)15-4-2/h3,9H,1,4-8H2,2H3
InchiKey: FRWJXBYBFQJBCX-UHFFFAOYSA-N
Formula: C11H17NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCC)CC1
Mol. weight [g/mol]: 211.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.14		Crippen Method
logp	0.974		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
rinpole	1761.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U361051&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

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