

Isonipecotic acid, N-acryloyl-, octyl ester

Inchi: InChI=1S/C17H29NO3/c1-3-5-6-7-8-9-14-21-17(20)15-10-12-18(13-11-15)16(19)4-2/h4,17-18,20-21
InchiKey: DDLUQKPKLNQCRI-UHFFFAOYSA-N
Formula: C17H29NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCCCCC)CC1
Mol. weight [g/mol]: 295.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	3.315		Crippen Method
mcvol	254.220	ml/mol	McGowan Method
rinpol	2395.00		NIST Webbook
rinpol	2395.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361057&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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