

Isonipecotic acid, N-acryloyl-, nonyl ester

Inchi: InChI=1S/C18H31NO3/c1-3-5-6-7-8-9-10-15-22-18(21)16-11-13-19(14-12-16)17(20)4-2/
InchiKey: YAMVWKFEAYGPQH-UHFFFAOYSA-N
Formula: C18H31NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCCCCCC)CC1
Mol. weight [g/mol]: 309.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	3.705		Crippen Method
mcvol	268.310	ml/mol	McGowan Method
rinpol	2504.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361058&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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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