

Isonipecotic acid, N-acryloyl-, hexyl ester

Inchi: InChI=1S/C15H25NO3/c1-3-5-6-7-12-19-15(18)13-8-10-16(11-9-13)14(17)4-2/h4,13H,2-
InchiKey: INUJGEIHANRHCR-UHFFFAOYSA-N
Formula: C15H25NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCC)CC1
Mol. weight [g/mol]: 267.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	2.534		Crippen Method
mcvol	226.040	ml/mol	McGowan Method
rinpola	2180.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U361055&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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