

Isonipecotic acid, N-acryloyl-, decyl ester

Inchi: InChI=1S/C19H33NO3/c1-3-5-6-7-8-9-10-11-16-23-19(22)17-12-14-20(15-13-17)18(21)4
InchiKey: CQNPAYCNPBCVLR-UHFFFAOYSA-N
Formula: C19H33NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCCCCCCCC)CC1
Mol. weight [g/mol]: 323.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	4.095		Crippen Method
mcvol	282.400	ml/mol	McGowan Method
rinpol	2606.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U361059&Units=SI>

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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