

Isonipecotic acid, N-acryloyl-, hexadecyl ester

Inchi: InChI=1S/C25H45NO3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-22-29-25(28)23-18-20-2
InchiKey: QJMQPLLROULEBC-UHFFFAOYSA-N
Formula: C25H45NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCCCCCCCCCCCCCC)CC1
Mol. weight [g/mol]: 407.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.00		Crippen Method
logp	6.436		Crippen Method
mcvol	366.940	ml/mol	McGowan Method
rinpol	3243.00		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=U361065&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

Latest version available from:

<https://www.chemeo.com/cid/41-487-6/Isonipecotic-acid-N-acryloyl-hexadecyl-ester.pdf>

Generated by Cheméo on 2024-04-26 08:55:52.324506513 +0000 UTC m=+16411001.245083829.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.