

Isonipectic acid, N-acryloyl-, tridecyl ester

Inchi: InChI=1S/C22H39NO3/c1-3-5-6-7-8-9-10-11-12-13-14-19-26-22(25)20-15-17-23(18-16-2
InchiKey: AMYCYGWXAADNHU-UHFFFAOYSA-N
Formula: C22H39NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCCCCCCCCCC)CC1
Mol. weight [g/mol]: 365.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.75		Crippen Method
logp	5.265		Crippen Method
mcvol	324.670	ml/mol	McGowan Method
rinpol	2921.00		NIST Webbook
rinpol	2921.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361062&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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