

Isonipecotic acid, N-acryloyl-, dodecyl ester

Inchi: InChI=1S/C21H37NO3/c1-3-5-6-7-8-9-10-11-12-13-18-25-21(24)19-14-16-22(17-15-19)2
InchiKey: DSOXBYVGSYQBNS-UHFFFAOYSA-N
Formula: C21H37NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCCCCCCCCCC)CC1
Mol. weight [g/mol]: 351.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	4.875		Crippen Method
mcvol	310.580	ml/mol	McGowan Method
rinpol	2806.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361061&Units=SI>
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>

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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