Isonipecotic acid, N-acryloyl-, undecyl ester

Inchi: InChI=1S/C20H35NO3/c1-3-5-6-7-8-9-10-11-12-17-24-20(23)18-13-15-21(16-14-18)19(2
InchiKey: ZIXCKGRYVNSZJW-UHFFFAOYSA-N
Formula: C20H35NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCCCCCCCC)CC1
Mol. weight [g/mol]: 337.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	4.485		Crippen Method
mcvol	296.490	ml/mol	McGowan Method
rinpol	2708.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361060&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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