Isonipecotic acid, N-acryloyl-, heptyl ester

Inchi: InChI=1S/C16H27NO3/c1-3-5-6-7-8-13-20-16(19)14-9-11-17(12-10-14)15(18)4-2/h4,14H
InchiKey: DKPWFWGUDABMQP-UHFFFAOYSA-N
Formula: C16H27NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCCCC)CC1
Mol. weight [g/mol]: 281.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.925		Crippen Method
mcvol	240.130	ml/mol	McGowan Method
rinpol	2290.00		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=U361056&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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