Isonipecotic acid, N-acryloyl-, pentyl ester

Inchi: InChI=1S/C14H23NO3/c1-3-5-6-11-18-14(17)12-7-9-15(10-8-12)13(16)4-2/h4,12H,2-3,5-
InchiKey: APZRMPGIRJVQCA-UHFFFAOYSA-N
Formula: C14H23NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCCC)CC1
Mol. weight [g/mol]: 253.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	2.144		Crippen Method
mcvol	211.950	ml/mol	McGowan Method
rinpol	2077.00		NIST Webbook

Sources

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=U361053&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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