

Isonipecotic acid, N-acryloyl-, butyl ester

Inchi: InChI=1S/C13H21NO3/c1-3-5-10-17-13(16)11-6-8-14(9-7-11)12(15)4-2/h4,11H,2-3,5-10H
InchiKey: PSYIPVSSPLMAPA-UHFFFAOYSA-N
Formula: C13H21NO3
SMILES: C=CC(=O)N1CCC(C(=O)OCCCC)CC1
Mol. weight [g/mol]: 239.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.98		Crippen Method
logp	1.754		Crippen Method
mcvol	197.860	ml/mol	McGowan Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361052&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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