

Isonipecotic acid, N-methacryloyl-, pentyl ester

Inchi: InChI=1S/C15H25NO3/c1-4-5-6-11-19-15(18)13-7-9-16(10-8-13)14(17)12(2)3/h13H,2,4-H
InchiKey: JABDRUIBWIPSIQ-UHFFFAOYSA-N
Formula: C15H25NO3
SMILES: C=C(C)C(=O)N1CCCC(C(=O)OCCCC)CC1
Mol. weight [g/mol]: 267.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	2.534		Crippen Method
mcvol	226.040	ml/mol	McGowan Method
rinpol	2086.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U360957&Units=SI>
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>

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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