Isonipecotic acid, N-methacryloyl-, octyl ester

Inchi: InChI=1S/C18H31NO3/c1-4-5-6-7-8-9-14-22-18(21)16-10-12-19(13-11-16)17(20)15(2)3/h
InchiKey: ZAZBKMONTFZAPM-UHFFFAOYSA-N
Formula: C18H31NO3
SMILES: C=C(C)C(=O)N1CCC(C(=O)OCCCCCCCC)CC1
Mol. weight [g/mol]: 309.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	3.705		Crippen Method
mcvol	268.310	ml/mol	McGowan Method
rinpol	2400.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360959&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