

Isonipectic acid, N-methacryloyl-, nonyl ester

Inchi: InChI=1S/C19H33NO3/c1-4-5-6-7-8-9-10-15-23-19(22)17-11-13-20(14-12-17)18(21)16(2)
InchiKey: TWNYCUFLEXNAEL-UHFFFAOYSA-N
Formula: C19H33NO3
SMILES: C=C(C)C(=O)N1CCC(C(=O)OCCCCCCCCC)CC1
Mol. weight [g/mol]: 323.47

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.49 | | Crippen Method |
| logp | 4.095 | | Crippen Method |
| mcvol | 282.400 | ml/mol | McGowan Method |
| rinpole | 2505.00 | | NIST Webbook |
| rinpole | 2505.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U360960&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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