

Isonipecotic acid, N-methacryloyl-, octadecyl ester

Inchi:	InChI=1S/C28H51NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-32-28(31)26-2
InchiKey:	VGMFRFLTRHMXFJ-UHFFFAOYSA-N
Formula:	C28H51NO3
SMILES:	C=C(C)C(=O)N1CCC(C(=O)OCCCCCCCCCCCCCCCCCC)CC1
Mol. weight [g/mol]:	449.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.26		Crippen Method
logp	7.606		Crippen Method
mcvol	409.210	ml/mol	McGowan Method
rinpola	3457.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360969&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
mcvola:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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