

Isonipectic acid, N-methacryloyl-, tridecyl ester

Inchi:	InChI=1S/C23H41NO3/c1-4-5-6-7-8-9-10-11-12-13-14-19-27-23(26)21-15-17-24(18-16-2
InchiKey:	LMCWODILWZDKGP-UHFFFAOYSA-N
Formula:	C23H41NO3
SMILES:	C=C(C)C(=O)N1CCC(C(=O)OCCCCCCCCCCCCC)CC1
Mol. weight [g/mol]:	379.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.16		Crippen Method
logp	5.655		Crippen Method
mcvol	338.760	ml/mol	McGowan Method
rmpol	2921.00		NIST Webbook
rmpol	2921.00		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=U360964&Units=SI

Legend

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

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