

Isonipectic acid, N-(3-methylbenzoyl)-, octyl ester

Inchi:	InChI=1S/C22H33NO3/c1-3-4-5-6-7-8-16-26-22(25)19-12-14-23(15-13-19)21(24)20-11-9
InchiKey:	RXUWFTGLIWMQAE-UHFFFAOYSA-N
Formula:	C22H33NO3
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C)c2)CC1
Mol. weight [g/mol]:	359.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	4.751		Crippen Method
mcvol	305.210	ml/mol	McGowan Method
rinpol	2991.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.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=U361103&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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