

Isonipectic acid, N-(2-methoxybenzoyl)-, isohexyl ester

Inchi:	InChI=1S/C20H29NO4/c1-15(2)7-6-14-25-20(23)16-10-12-21(13-11-16)19(22)17-8-4-5-9
InchiKey:	QFQSFEZRUCJLP-UHFFFAOYSA-N
Formula:	C20H29NO4
SMILES:	COc1ccccc1C(=O)N1CCC(C(=O)OCCCC(C)C)CC1
Mol. weight [g/mol]:	347.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.527		Crippen Method
mcvol	282.900	ml/mol	McGowan Method
rinpol	2758.00		NIST Webbook
rinpol	2758.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

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