

Isonipectic acid, N-(4-ethylbenzoyl)-, octyl ester

Inchi:	InChI=1S/C23H35NO3/c1-3-5-6-7-8-9-18-27-23(26)21-14-16-24(17-15-21)22(25)20-12-1
InchiKey:	KNFVQHBMLKFMMM-UHFFFAOYSA-N
Formula:	C23H35NO3
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(CC)cc2)CC1
Mol. weight [g/mol]:	373.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	5.005		Crippen Method
mcvol	319.300	ml/mol	McGowan Method
rinpol	3112.00		NIST Webbook
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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=U361145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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