

Isonipectic acid, N-(4-butylbenzoyl)-, butyl ester

Inchi:	InChI=1S/C21H31NO3/c1-3-5-7-17-8-10-18(11-9-17)20(23)22-14-12-19(13-15-22)21(24)
InchiKey:	ZEGNJVZEWRXQPV-UHFFFAOYSA-N
Formula:	C21H31NO3
SMILES:	CCCCOC(=O)C1CCN(C(=O)c2ccc(CCCC)cc2)CC1
Mol. weight [g/mol]:	345.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	4.225		Crippen Method
mcvol	291.120	ml/mol	McGowan Method
rinpol	2883.00		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=U361130&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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