

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

Inchi:	InChI=1S/C19H27NO3/c1-3-5-6-15-7-9-16(10-8-15)18(21)20-13-11-17(12-14-20)19(22)2
InchiKey:	SSTYJBRTGNVXQT-UHFFFAOYSA-N
Formula:	C19H27NO3
SMILES:	CCCCc1ccc(C(=O)N2CCC(C(=O)OCC)CC2)cc1
Mol. weight [g/mol]:	317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	3.444		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinsol	2669.00		NIST Webbook
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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=U361127&Units=SI

Legend

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

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