

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

Inchi:	InChI=1S/C20H29NO3/c1-3-5-6-15-24-20(23)18-11-13-21(14-12-18)19(22)17-9-7-16(4-2
InchiKey:	KDWXKLBHXLLKDL-UHFFFAOYSA-N
Formula:	C20H29NO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2ccc(CC)cc2)CC1
Mol. weight [g/mol]:	331.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	3.835		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinsol	2772.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361141&Units=SI
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

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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