

Isonipecotic acid, N-(4-ethylbenzoyl)-, isoheptyl ester

Inchi:	InChI=1S/C21H31NO3/c1-4-17-7-9-18(10-8-17)20(23)22-13-11-19(12-14-22)21(24)25-15
InchiKey:	HAQSGNJIUNUOSZ-UHFFFAOYSA-N
Formula:	C21H31NO3
SMILES:	CCc1ccc(C(=O)N2CCC(C(=O)OCCCC(C)C)CC2)cc1
Mol. weight [g/mol]:	345.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Crippen Method
logp	4.081		Crippen Method
mcvol	291.120	ml/mol	McGowan Method
rinpol	2837.00		NIST Webbook
rinpol	2837.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361142&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
rinpol:	Non-polar retention indices

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