

Pipecolic acid, N-isobutoxycarbonyl-, decyl ester

Inchi:	InChI=1S/C21H39NO4/c1-4-5-6-7-8-9-10-13-16-25-20(23)19-14-11-12-15-22(19)21(24)2
InchiKey:	FWZMHEJXOOINFT-UHFFFAOYSA-N
Formula:	C21H39NO4
SMILES:	CCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]:	369.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.65		Crippen Method
logp	5.317		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U393023&Units=SI

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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<https://www.chemeo.com/cid/94-601-0/Pipecolic-acid-N-isobutoxycarbonyl-decyl-ester.pdf>

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