

Pipecolic acid, N-octyloxycarbonyl-, isobutyl ester

Inchi:	InChI=1S/C19H35NO4/c1-4-5-6-7-8-11-14-23-19(22)20-13-10-9-12-17(20)18(21)24-15-1
InchiKey:	PIAJMJWLBSYJY-UHFFFAOYSA-N
Formula:	C19H35NO4
SMILES:	CCCCCCCCOC(=O)N1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	341.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	4.537		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
rinpola	2306.00		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=U393124&Units=SI

Legend

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

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