

Pipecolylpipecolic acid, N-ethoxycarbonyl-, hexyl ester

Inchi:	InChI=1S/C21H36N2O5/c1-3-5-6-11-16-28-20(25)18-13-8-9-14-22(18)19(24)17-12-7-10
InchiKey:	KTVURSPFTIQNHY-UHFFFAOYSA-N
Formula:	C21H36N2O5
SMILES:	CCCCCOC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCC
Mol. weight [g/mol]:	396.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	3.502		Crippen Method
mcvol	321.440	ml/mol	McGowan Method
rinpola	2779.00		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=U393084&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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