

Pipecolic acid, N-hexyloxycarbonyl-, pentyl ester

Inchi:	InChI=1S/C18H33NO4/c1-3-5-7-11-15-23-18(21)19-13-9-8-12-16(19)17(20)22-14-10-6-4
InchiKey:	VZZUMZFDCIAPOY-UHFFFAOYSA-N
Formula:	C18H33NO4
SMILES:	CCCCCOC(=O)N1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]:	327.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	4.291		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
rmpol	2265.00		NIST Webbook
rmpol	2265.00		NIST Webbook

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=U393111&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/99-361-2/Pipecolic-acid-N-hexyloxycarbonyl-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-29 11:57:38.489231084 +0000 UTC m=+16681107.409808395.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.