

Pipecolic acid, N-propoxycarbonyl-, hexyl ester

Inchi:	InChI=1S/C16H29NO4/c1-3-5-6-9-13-20-15(18)14-10-7-8-11-17(14)16(19)21-12-4-2/h14
InchiKey:	CAVJDOYMACUTNC-UHFFFAOYSA-N
Formula:	C16H29NO4
SMILES:	CCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]:	299.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	3.511		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinsol	2076.00		NIST Webbook
rinsol	2076.00		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=U392997&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/116-657-4/Pipecolic-acid-N-propoxycarbonyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-29 12:17:16.075609483 +0000 UTC m=+16682284.996186795.

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