

Pipecolic acid, N-hexyloxycarbonyl-, heptyl ester

Inchi:	InChI=1S/C20H37NO4/c1-3-5-7-9-13-16-24-19(22)18-14-10-11-15-21(18)20(23)25-17-12
InchiKey:	MYSBCSVOAKWDJN-UHFFFAOYSA-N
Formula:	C20H37NO4
SMILES:	CCCCCCCCOC(=O)C1CCCCN1C(=O)OCCCCC
Mol. weight [g/mol]:	355.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.47		Crippen Method
logp	5.071		Crippen Method
mcvol	306.660	ml/mol	McGowan Method
rinpol	2482.00		NIST Webbook
rinpol	2482.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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