

Pipecolic acid, N-hexyloxycarbonyl-, dodecyl ester

Inchi:	InChI=1S/C25H47NO4/c1-3-5-7-9-10-11-12-13-14-18-21-29-24(27)23-19-15-16-20-26(28)
InchiKey:	FOJKVPHGJWIYKE-UHFFFAOYSA-N
Formula:	C25H47NO4
SMILES:	CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCCCC
Mol. weight [g/mol]:	425.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	7.022		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
rinpola	2999.00		NIST Webbook
rinpola	2999.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393117&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
rinpola:	Non-polar retention indices

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