

Pipecolic acid, N-octyloxycarbonyl-, pentadecyl ester

Inchi:	InChI=1S/C30H57NO4/c1-3-5-7-9-11-12-13-14-15-16-17-19-22-26-34-29(32)28-24-20-2
InchiKey:	DKWPZWXTCBETGL-UHFFFAOYSA-N
Formula:	C30H57NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCCN1C(=O)OCCCCCCCC
Mol. weight [g/mol]:	495.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.66		Crippen Method
logp	8.972		Crippen Method
mcvol	447.560	ml/mol	McGowan Method
rinpola	3467.00		NIST Webbook
rinpola	3467.00		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=U393136&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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