

Pipecolic acid, N-butoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C18H33NO4/c1-3-5-7-8-11-15-22-17(20)16-12-9-10-13-19(16)18(21)23-14-6-4
InchiKey: HHQFIELYXPUPSQ-UHFFFAOYSA-N
Formula: C18H33NO4
SMILES: CCCCCCOC(=O)C1CCCCN1C(=O)OCCCC
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
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393053&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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