

Pipecoly pipecolic acid, N-butoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C24H42N2O5/c1-3-5-7-8-13-19-30-23(28)21-15-10-11-16-25(21)22(27)20-14-9
InchiKey: KRNYWKJIDFJROH-UHFFFAOYSA-N
Formula: C24H42N2O5
SMILES: CCCCCCOC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCCCC
Mol. weight [g/mol]: 438.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Crippen Method
logp	4.672		Crippen Method
mcvol	363.710	ml/mol	McGowan Method
rinpole	3003.00		NIST Webbook
rinpole	3003.00		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=U393068&Units=SI>

Legend

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

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