

Pipecolylpipecolic acid, N-butoxycarbonyl-, octyl ester

Inchi: InChI=1S/C25H44N2O5/c1-3-5-7-8-9-14-20-31-24(29)22-16-11-12-17-26(22)23(28)21-15
InchiKey: GKYGEGYTYPFXIU-UHFFFAOYSA-N
Formula: C25H44N2O5
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)C1CCCN1C(=O)OCCCC
Mol. weight [g/mol]: 452.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	5.062		Crippen Method
mcvol	377.800	ml/mol	McGowan Method
rinpole	3108.00		NIST Webbook
rinpole	3108.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393069&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
rinpole: Non-polar retention indices

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