

Pipecolylpipecolic acid, N-ethoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C19H32N2O5/c1-4-25-19(24)21-12-8-5-9-15(21)17(22)20-11-7-6-10-16(20)18
InchiKey: VLIHUWBWTARHIY-UHFFFAOYSA-N
Formula: C19H32N2O5
SMILES: CCOC(=O)N1CCCCC1C(=O)N1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	2.578		Crippen Method
mcvol	293.260	ml/mol	McGowan Method
rinpol	2539.00		NIST Webbook
rinpol	2539.00		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=U393081&Units=SI>

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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