

Isonipecotic acid, N-(5-chlorovaleryl)-, isobutyl ester

Inchi: InChI=1S/C15H26ClNO3/c1-12(2)11-20-15(19)13-6-9-17(10-7-13)14(18)5-3-4-8-16/h12-14,17-19,20H,1H3
InchiKey: HQGBJNUQDJBQDJ-UHFFFAOYSA-N
Formula: C15H26ClNO3
SMILES: CC(C)COC(=O)C1CCN(C(=O)CCCCCl)CC1
Mol. weight [g/mol]: 303.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	2.833		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
rinpol	2401.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361004&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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