

Isonipecotic acid, N-(3-chloropropionyl)-, butyl ester

Inchi: InChI=1S/C13H22ClNO3/c1-2-3-10-18-13(17)11-5-8-15(9-6-11)12(16)4-7-14/h11H,2-10H
InchiKey: HUVXMECXTUBTRZ-UHFFFAOYSA-N
Formula: C13H22ClNO3
SMILES: CCCOC(=O)C1CCN(C(=O)CCCl)CC1
Mol. weight [g/mol]: 275.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	2.197		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
rinpol	2099.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U360943&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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