

Isonipectic acid, N-(5-chlorovaleryl)-, butyl ester

Inchi:	InChI=1S/C15H26ClNO3/c1-2-3-12-20-15(19)13-7-10-17(11-8-13)14(18)6-4-5-9-16/h13H
InchiKey:	CQQGLUPSZNHMQD-UHFFFAOYSA-N
Formula:	C15H26ClNO3
SMILES:	CCCCOC(=O)C1CCN(C(=O)CCCCCl)CC1
Mol. weight [g/mol]:	303.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.977		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
rinpola	2449.00		NIST Webbook

Sources

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=U361005&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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