

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

Inchi: InChI=1S/C16H28ClNO3/c1-2-3-4-5-6-13-21-16(20)14-8-11-18(12-9-14)15(19)7-10-17/h
InchiKey: SLVNRHDNQITEHG-UHFFFAOYSA-N
Formula: C16H28ClNO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)CCCl)CC1
Mol. weight [g/mol]: 317.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	3.367		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		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=U360946&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/56-196-3/Isonipecotic-acid-N-3-chloropropionyl-heptyl-ester.pdf>

Generated by Cheméo on 2024-04-18 01:28:27.74508386 +0000 UTC m=+15692956.665661172.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.