

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

Inchi: InChI=1S/C26H48ClNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-31-26(30)24-18-2
InchiKey: IYMLZRTXSMSRQI-UHFFFAOYSA-N
Formula: C₂₆H₄₈ClNO₃
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CCCl)CC1
Mol. weight [g/mol]: 458.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.72		Crippen Method
logp	7.268		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
rinpol	3474.00		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=U360956&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

Latest version available from:

<https://www.chemeo.com/cid/14-650-4/Isonipecotic-acid-N-3-chloropropionyl-heptadecyl-ester.pdf>

Generated by Cheméo on 2025-12-05 20:12:47.43526535 +0000 UTC m=+4713764.965306015.

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