1,2,3,4-Tetrahydroquinoline, N-(3-chloropropyl)-

Inchi: InChI=1S/C12H16ClN/c13-8-4-10-14-9-3-6-11-5-1-2-7-12(11)14/h1-2,5,7H,3-4,6,8-10H2
InchiKey: LOGKGIGCOMGMFU-UHFFFAOYSA-N
Formula: C12H16ClN
SMILES: ClCCCN1CCCc2ccccc21
Mol. weight [g/mol]: 209.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	3.068		Crippen Method
mcvol	167.540	ml/mol	McGowan Method
rinpol	1825.00		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=U380696&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
rinpol: Non-polar retention indices