

Thiophene-2-carboxamide, N-(3-chlorophenyl)-

Inchi: InChI=1S/C11H8ClNOS/c12-8-3-1-4-9(7-8)13-11(14)10-5-2-6-15-10/h1-7H,(H,13,14)
InchiKey: FHTIWIPMVNMNHO-UHFFFAOYSA-N
Formula: C11H8ClNOS
SMILES: O=C(Nc1cccc(Cl)c1)c1cccs1
Mol. weight [g/mol]: 237.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	3.654		Crippen Method
mcvol	162.770	ml/mol	McGowan Method
rinpole	2151.00		NIST Webbook
rinpole	2151.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307070&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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