Acetamide, N-(3-chlorophenyl)-2-(2-thienyl)-

Inchi: InChI=1S/C12H10ClNOS/c13-9-3-1-4-10(7-9)14-12(15)8-11-5-2-6-16-11/h1-7H,8H2,(H,1
InchiKey: RTZYPCPHOITSSY-UHFFFAOYSA-N
Formula: C12H10ClNOS
SMILES: O=C(Cc1cccs1)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 251.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	3.583		Crippen Method
mcvol	176.860	ml/mol	McGowan Method
rinpol	2147.00		NIST Webbook
rinpol	2147.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U306903&Units=SI
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

Legend

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

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