Propanamide, N-(3-chlorophenyl)-2,2-dimethyl-

Inchi: InChI=1S/C11H14ClNO/c1-11(2,3)10(14)13-9-6-4-5-8(12)7-9/h4-7H,1-3H3,(H,13,14)
InchiKey: OGOQXGKPTWSHPS-UHFFFAOYSA-N
Formula: C11H14ClNO
SMILES: CC(C)(C)C(O)=Nc1cccc(Cl)c1
Mol. weight [g/mol]: 211.69

Physical Properties

Property code	Value	Unit	Source
hf	-149.60	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.974		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
tb	685.68	K	Joback Method
tc	909.20	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307196&Units=SI

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature