

Propanamide, N-(3-chlorophenyl)-3-phenyl-

Inchi: InChI=1S/C15H14ClNO/c16-13-7-4-8-14(11-13)17-15(18)10-9-12-5-2-1-3-6-12/h1-8,11H
InchiKey: WNWRTBIACAYQKW-UHFFFAOYSA-N
Formula: C15H14ClNO
SMILES: OC(Cc1ccccc1)=Nc1cccc(Cl)c1
Mol. weight [g/mol]: 259.73

Physical Properties

Property code	Value	Unit	Source
hf	13.12	kJ/mol	Joback Method
hvap	78.66	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.561		Crippen Method
mcvol	198.480	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	807.11	K	Joback Method
tc	1042.39	K	Joback Method

Sources

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=U308116&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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