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

Inchi: InChI=1S/C14H12ClNO/c15-12-7-4-8-13(10-12)16-14(17)9-11-5-2-1-3-6-11/h1-8,10H,9H
InchiKey: GAWITMMQHFGOMV-UHFFFAOYSA-N
Formula: C14H12ClNO
SMILES: O=C(Cc1ccccc1)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 245.70

Physical Properties

Property code	Value	Unit	Source
gf	230.73	kJ/mol	Joback Method
hf	54.45	kJ/mol	Joback Method
hfus	30.60	kJ/mol	Joback Method
hvap	69.54	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.521		Crippen Method
mcvol	184.390	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	2147.00		NIST Webbook
rinpol	2147.00		NIST Webbook
tb	719.53	K	Joback Method
tc	966.46	K	Joback Method
tf	445.41	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.51	J/mol×K	719.53	Joback Method
cpg	477.98	J/mol×K	760.69	Joback Method
cpg	490.29	J/mol×K	801.84	Joback Method
cpg	501.50	J/mol×K	843.00	Joback Method
cpg	511.70	J/mol×K	884.15	Joback Method
cpg	520.97	J/mol×K	925.31	Joback Method
cpg	529.40	J/mol×K	966.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307143&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume