2-Butenamide, N-(3-chlorophenyl)-3-methyl-

Inchi: InChI=1S/C11H12ClNO/c1-8(2)6-11(14)13-10-5-3-4-9(12)7-10/h3-7H,1-2H3,(H,13,14)
InchiKey: DYNVGFUQFOJQAY-UHFFFAOYSA-N
Formula: C11H12ClNO
SMILES: CC(C)=CC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 209.67

Physical Properties

Property code	Value	Unit	Source
gf	164.73	kJ/mol	Joback Method
hf	-12.73	kJ/mol	Joback Method
hfus	27.68	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.245		Crippen Method
mcvol	161.580	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1843.00		NIST Webbook
tb	628.25	K	Joback Method
tc	857.64	K	Joback Method
tf	366.14	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.63	J/mol×K	628.25	Joback Method
cpg	388.53	J/mol×K	666.48	Joback Method
cpg	400.52	J/mol×K	704.71	Joback Method
cpg	411.64	J/mol×K	742.95	Joback Method
cpg	421.95	J/mol×K	781.18	Joback Method
cpg	431.53	J/mol×K	819.41	Joback Method
cpg	440.43	J/mol×K	857.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307269&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