N-(2-Chloro-4-methylphenyl)acetamide

Other names: Acetamide, N-(2-chloro-4-methylphenyl)-
Inchi: InChI=1S/C9H10ClNO/c1-6-3-4-9(8(10)5-6)11-7(2)12/h3-5H,1-2H3,(H,11,12)
InchiKey: PSGFNVAAKYVOAT-UHFFFAOYSA-N
Formula: C9H10ClNO
SMILES: CC(=O)Nc1ccc(C)cc1Cl
Mol. weight [g/mol]: 183.63

Physical Properties

Property code	Value	Unit	Source
gf	66.59	kJ/mol	Joback Method
hf	-90.35	kJ/mol	Joback Method
hfus	23.22	kJ/mol	Joback Method
hvap	56.80	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.607		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	1531.00		NIST Webbook
tb	583.43	K	Joback Method
tc	808.69	K	Joback Method
tf	375.16	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.78	J/mol×K	583.43	Joback Method
cpg	313.33	J/mol×K	620.97	Joback Method
cpg	324.14	J/mol×K	658.52	Joback Method
cpg	334.25	J/mol×K	696.06	Joback Method
cpg	343.67	J/mol×K	733.60	Joback Method
cpg	352.44	J/mol×K	771.15	Joback Method
cpg	360.58	J/mol×K	808.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373202&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

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