N-Acetyl-N-(2-chloro-4-methylphenyl)acetamide

Other names: Acetamide, N-acetyl-N-(4-chloro-2-methylphenyl)-
Inchi: InChI=1S/C11H12ClNO2/c1-7-4-5-11(10(12)6-7)13(8(2)14)9(3)15/h4-6H,1-3H3
InchiKey: VNYHCBVBVVCJOW-UHFFFAOYSA-N
Formula: C11H12ClNO2
SMILES: CC(=O)N(C(C)=O)c1ccc(C)cc1Cl
Mol. weight [g/mol]: 225.67

Physical Properties

Property code	Value	Unit	Source
gf	-24.10	kJ/mol	Joback Method
hf	-230.15	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	63.60	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.548		Crippen Method
mcvol	167.450	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
tb	645.33	K	Joback Method
tc	867.05	K	Joback Method
tf	427.44	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.84	J/mol×K	645.33	Joback Method
cpg	411.26	J/mol×K	682.28	Joback Method
cpg	422.82	J/mol×K	719.24	Joback Method
cpg	433.57	J/mol×K	756.19	Joback Method
cpg	443.52	J/mol×K	793.14	Joback Method
cpg	452.74	J/mol×K	830.10	Joback Method
cpg	461.24	J/mol×K	867.05	Joback Method

Sources

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=U373203&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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