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

Inchi: InChI=1S/C10H10ClNO3/c1-7(13)15-6-10(14)12-9-4-2-3-8(11)5-9/h2-5H,6H2,1H3,(H,12,
InchiKey: ZTOFIGAKFYAJPE-UHFFFAOYSA-N
Formula: C10H10ClNO3
SMILES: CC(=O)OCC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 227.64

Physical Properties

Property code	Value	Unit	Source
gf	-149.28	kJ/mol	Joback Method
hf	-344.32	kJ/mol	Joback Method
hfus	28.99	kJ/mol	Joback Method
hvap	67.52	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.842		Crippen Method
mcvol	159.230	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1814.00		NIST Webbook
tb	677.62	K	Joback Method
tc	901.54	K	Joback Method
tf	446.07	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.28	J/mol×K	677.62	Joback Method
cpg	396.30	J/mol×K	714.94	Joback Method
cpg	406.52	J/mol×K	752.26	Joback Method
cpg	415.96	J/mol×K	789.58	Joback Method
cpg	424.64	J/mol×K	826.90	Joback Method
cpg	432.57	J/mol×K	864.22	Joback Method
cpg	439.76	J/mol×K	901.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307092&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