Acetophenone, 5'-chloro-2'-nitro-

Inchi: InChI=1S/C8H6ClNO3/c1-5(11)7-4-6(9)2-3-8(7)10(12)13/h2-4H,1H3
InchiKey: HVXQVXNQKCPSLH-UHFFFAOYSA-N
Formula: C8H6ClNO3
SMILES: CC(=O)c1cc(Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 199.59
CAS: 18640-60-3

Physical Properties

Property code	Value	Unit	Source
gf	4.33	kJ/mol	Joback Method
hf	-133.94	kJ/mol	Joback Method
hfus	26.90	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.451		Crippen Method
mcvol	131.050	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	662.22	K	Joback Method
tc	917.82	K	Joback Method
tf	454.84	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.22	J/mol×K	662.22	Joback Method
cpg	304.78	J/mol×K	704.82	Joback Method
cpg	313.53	J/mol×K	747.42	Joback Method
cpg	321.52	J/mol×K	790.02	Joback Method
cpg	328.78	J/mol×K	832.62	Joback Method
cpg	335.35	J/mol×K	875.22	Joback Method
cpg	341.26	J/mol×K	917.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18640603&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume