2,6-Dichloroacetophenone

Other names: Ethanone, 1-(2,6-dichlorophenyl)-
1-(2,6-dichlorophenyl)ethan-1-one
Inchi: InChI=1S/C8H6Cl2O/c1-5(11)8-6(9)3-2-4-7(8)10/h2-4H,1H3
InchiKey: HYBDSXBLGCQKRE-UHFFFAOYSA-N
Formula: C8H6Cl2O
SMILES: CC(=O)c1c(Cl)cccc1Cl
Mol. weight [g/mol]: 189.04
CAS: 2040-05-3

Physical Properties

Property code	Value	Unit	Source
gf	-43.15	kJ/mol	Joback Method
hf	-138.92	kJ/mol	Joback Method
hfus	19.73	kJ/mol	Joback Method
hvap	52.52	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.196		Crippen Method
mcvol	125.870	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	547.81	K	Joback Method
tc	782.69	K	Joback Method
tf	341.15	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.65	J/mol×K	547.81	Joback Method
cpg	278.97	J/mol×K	743.54	Joback Method
cpg	271.89	J/mol×K	704.39	Joback Method
cpg	264.24	J/mol×K	665.25	Joback Method
cpg	256.00	J/mol×K	626.10	Joback Method
cpg	247.15	J/mol×K	586.96	Joback Method
cpg	285.50	J/mol×K	782.69	Joback Method

dvisc	0.0002927	Pa×s	547.81	Joback Method
dvisc	0.0003553	Pa×s	513.37	Joback Method
dvisc	0.0004435	Pa×s	478.92	Joback Method
dvisc	0.0005730	Pa×s	444.48	Joback Method
dvisc	0.0007729	Pa×s	410.04	Joback Method
dvisc	0.0011014	Pa×s	375.59	Joback Method
dvisc	0.0016858	Pa×s	341.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2040053&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
dvisc:	Dynamic viscosity
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