3,5-Dichloro-2-hydroxyacetophenone

Other names:	Ethanone, 1-(3,5-dichloro-2-hydroxyphenyl)-
	Acetophenone, 3',5'-dichloro-2'-hydroxy-
	2'-Hydroxy-3',5'-dichloroacetophenone
	2-Acetyl-4,6-dichlorophenol
	3',5'-Dichloro-2'-hydroxyacetophenone
	4,6-Dichloro-2-acetylphenol
	1-(3,5-Dichloro-2-hydroxy-phenyl)-ethanone
Inchi:	InChI=1S/C8H6Cl2O2/c1-4(11)6-2-5(9)3-7(10)8(6)12/h2-3,12H,1H3
InchiKey:	CJFYGRLJDKWMDI-UHFFFAOYSA-N
Formula:	C8H6Cl2O2
SMILES:	CC(=O)c1cc(Cl)cc(Cl)c1O
Mol. weight [g/mol]:	205.04
CAS:	3321-92-4

Physical Properties

Property code	Value	Unit	Source
gf	-197.77	kJ/mol	Joback Method
hf	-316.23	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.902		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	628.43	K	Joback Method
tc	873.32	K	Joback Method
tf	452.87	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.54	J/mol×K	628.43	Joback Method
cpg	284.67	J/mol×K	669.25	Joback Method

cpg	292.20	J/mol×K	710.06	Joback Method
cpg	299.21	J/mol×K	750.88	Joback Method
cpg	305.77	J/mol×K	791.69	Joback Method
cpg	311.97	J/mol×K	832.51	Joback Method
cpg	317.90	J/mol×K	873.32	Joback Method
dvisc	0.0005001	Pa×s	452.87	Joback Method
dvisc	0.0002888	Pa×s	482.13	Joback Method
dvisc	0.0001776	Pa×s	511.39	Joback Method
dvisc	0.0001151	Pa×s	540.65	Joback Method
dvisc	0.0000780	Pa×s	569.91	Joback Method
dvisc	0.0000549	Pa×s	599.17	Joback Method
dvisc	0.0000400	Pa×s	628.43	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=C3321924&Units=SI

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