2,2-DICHLOROACETOPHENONE

Other names: 2,2-Dichloroacetophenone
«omega»,«omega»-Dichloroacetophenone
Acetophenone, 2,2-dichloro-
Ethanone, 2,2-dichloro-1-phenyl-
Phenacylidene chloride
1,1-Dichloroacetophenone
Inchi: InChI=1S/C8H6Cl2O/c9-8(10)7(11)6-4-2-1-3-5-6/h1-5,8H
InchiKey: CERJZAHSUZVMCH-UHFFFAOYSA-N
Formula: C8H6Cl2O
SMILES: O=C(c1ccccc1)C(Cl)Cl
Mol. weight [g/mol]: 189.04

Physical Properties

Property code	Value	Unit	Source
af	0.4008		Cheméo Relay (1.0)
gf	-26.33	kJ/mol	Joback Method
hf	-122.34	kJ/mol	Cheméo Relay (1.0)
hfus	16.99	kJ/mol	Joback Method
hvap	67.22	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-2.72		Cheméo Relay (1.0)
logp	2.673		Crippen Method
mcvol	125.870	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
tb	522.20	K	NIST Webbook
tc	763.75	K	Cheméo Relay (1.0)
tf	333.25	K	Cheméo Relay (1.0)
vc	0.443	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.85	J/mol×K	537.41	Joback Method
cpg	250.36	J/mol×K	577.08	Joback Method

cpg	260.03	J/mol×K	616.75	Joback Method
cpg	268.93	J/mol×K	656.42	Joback Method
cpg	277.08	J/mol×K	696.09	Joback Method
cpg	284.53	J/mol×K	735.76	Joback Method
cpg	291.33	J/mol×K	775.44	Joback Method
dvisc	0.0036093	Pa×s	301.11	Joback Method
dvisc	0.0018614	Pa×s	340.49	Joback Method
dvisc	0.0011013	Pa×s	379.88	Joback Method
dvisc	0.0007191	Pa×s	419.26	Joback Method
dvisc	0.0005052	Pa×s	458.64	Joback Method
dvisc	0.0003753	Pa×s	498.03	Joback Method
dvisc	0.0002912	Pa×s	537.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.20	K	1.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2648615&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume