

«alpha»,«alpha»-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
CAS:	2648-61-5

Physical Properties

Property code	Value	Unit	Source
gf	-26.33	kJ/mol	Joback Method
hf	-121.26	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	50.81	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
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	775.44	K	Joback Method
tf	301.11	K	Joback Method
vc	0.473	m3/kmol	Joback Method

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

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=C2648615&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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