4,4'-Dichlorobenzophenone

Other names:	Methanone, bis(4-chlorophenyl)-
	Benzophenone, 4,4'-dichloro-
	p,p'-Dichlorobenzophenone
	Bis(4-chlorophenyl) ketone
	DBP
	DCBP
	Di(p-Chlorophenyl)ketone
	DCB
	USAF DO-4
	p-Dichlorobenzophenone
	DBP (degradation product)
	NSC 8787
	p,p-Dichlorobenzophenone
	Dichloro-4,4'-dibenzophenone
Inchi:	InChI=1S/C13H8Cl2O/c14-11-5-1-9(2-6-11)13(16)10-3-7-12(15)8-4-10/h1-8H
InchiKey:	OKISUZLXOYGIFP-UHFFFAOYSA-N
Formula:	C13H8Cl2O
SMILES:	O=C(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	251.11
CAS:	90-98-2

Physical Properties

Property code	Value	Unit	Source
gf	111.36	kJ/mol	Joback Method
hf	-5.59	kJ/mol	Joback Method
hfus	26.72	kJ/mol	Joback Method
hsub	117.50 ± 0.30	kJ/mol	NIST Webbook
hvap	65.92	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.224		Crippen Method
mcvol	172.560	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	2014.00		NIST Webbook
rinpol	2018.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1979.00		NIST Webbook
tb	626.20	K	NIST Webbook

tc	948.38	K	Joback Method
tf	420.00 ± 0.20	K	NIST Webbook
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.24	J/mol×K	688.89	Joback Method
cpg	399.33	J/mol×K	732.14	Joback Method
cpg	410.32	J/mol×K	775.39	Joback Method
cpg	420.28	J/mol×K	818.64	Joback Method
cpg	429.27	J/mol×K	861.88	Joback Method
cpg	437.38	J/mol×K	905.13	Joback Method
cpg	444.68	J/mol×K	948.38	Joback Method
dvisc	0.0005279	Pa×s	512.24	Joback Method
dvisc	0.0007755	Pa×s	468.08	Joback Method
dvisc	0.0012341	Pa×s	423.92	Joback Method
dvisc	0.0003820	Pa×s	556.41	Joback Method
dvisc	0.0002899	Pa×s	600.57	Joback Method
dvisc	0.0002285	Pa×s	644.73	Joback Method
dvisc	0.0001857	Pa×s	688.89	Joback Method
hfust	30.12	kJ/mol	420.00	NIST Webbook
hfust	30.12	kJ/mol	420.00	NIST Webbook
hfust	21.65	kJ/mol	338.40	NIST Webbook
hsubt	114.50 ± 0.30	kJ/mol	358.00	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=C90982&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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume