Hexachloroacetone

Other names:	2-Propanone, 1,1,1,3,3,3-hexachloro-
	Bis(trichloromethyl) ketone
	Hexachloropropanone
	HCA
	Kureha HCA
	1,1,1,3,3,3-Hexachloro-2-propanone
	1,1,1,3,3,3-Hexachloropropanone
	2-Propanone, hexachloro-
	Hexachloro-2-propanone
	Acetone, hexachloro-
	GC-1106
	Perchloro-2-propanone
	HCA weedkiller
	UN 2661
	NSC 6852
	Perchloroacetone
Inchi:	InChI=1S/C3Cl6O/c4-2(5,6)1(10)3(7,8)9
InchiKey:	DOJXGHGHTWFZHK-UHFFFAOYSA-N
Formula:	C3Cl6O
SMILES:	O=C(C(Cl)(Cl)Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	264.75
CAS:	116-16-5

Physical Properties

Property code	Value	Unit	Source
gf	-220.44	kJ/mol	Joback Method
hf	-329.77	kJ/mol	Joback Method
hfus	15.48	kJ/mol	Joback Method
hvap	52.74	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.296		Crippen Method
mcvol	128.140	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1138.00		NIST Webbook
tb	476.20	K	NIST Webbook
tc	792.64	K	Joback Method

tf	357.86	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.13	J/mol×K	666.33	Joback Method
cpg	212.00	J/mol×K	792.64	Joback Method
cpg	210.79	J/mol×K	750.54	Joback Method
cpg	209.20	J/mol×K	708.43	Joback Method
cpg	197.15	J/mol×K	540.03	Joback Method
cpg	201.21	J/mol×K	582.13	Joback Method
cpg	204.50	J/mol×K	624.23	Joback Method
dvisc	0.0003726	Pa×s	540.03	Joback Method
dvisc	0.0009002	Pa×s	448.94	Joback Method
dvisc	0.0006463	Pa×s	479.31	Joback Method
dvisc	0.0004827	Pa×s	509.67	Joback Method
dvisc	0.0034078	Pa×s	357.86	Joback Method
dvisc	0.0020399	Pa×s	388.22	Joback Method
dvisc	0.0013155	Pa×s	418.58	Joback Method
hfust	8.38	kJ/mol	147.70	NIST Webbook
hvapt	23.10	kJ/mol	229.00	NIST Webbook
hvapt	22.30	kJ/mol	298.50	NIST Webbook
hvapt	23.60	kJ/mol	220.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.20	K	0.80	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116165&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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume