

2-Propanone, 1,1,1,3,3-pentachloro-

Other names:	Pentachloroacetone 1,1,1,3,3-Pentachloropropanone 2-Propanone, pentachloro- Pentachloropropanone
Inchi:	InChI=1S/C3HCl5O/c4-2(5)1(9)3(6,7)8/h2H
InchiKey:	RVSIFWBAGVMQKT-UHFFFAOYSA-N
Formula:	C3HCl5O
SMILES:	O=C(C(Cl)Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	230.30
CAS:	1768-31-6

Physical Properties

Property code	Value	Unit	Source
gf	-213.79	kJ/mol	Joback Method
hf	-310.56	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	49.26	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.729		Crippen Method
mcvol	115.900	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	465.20	K	NIST Webbook
tc	742.44	K	Joback Method
tf	310.52	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.81	J/molxK	505.39	Joback Method
cpg	194.91	J/molxK	702.93	Joback Method
cpg	192.23	J/molxK	663.42	Joback Method
cpg	189.13	J/molxK	623.91	Joback Method
cpg	185.56	J/molxK	584.41	Joback Method

cpg	181.47	J/mol×K	544.90	Joback Method
cpg	197.21	J/mol×K	742.44	Joback Method
dvisc	0.0004169	Paxs	505.39	Joback Method
dvisc	0.0005452	Paxs	472.91	Joback Method
dvisc	0.0007418	Paxs	440.43	Joback Method
dvisc	0.0010598	Paxs	407.95	Joback Method
dvisc	0.0016107	Paxs	375.48	Joback Method
dvisc	0.0026498	Paxs	343.00	Joback Method
dvisc	0.0048378	Paxs	310.52	Joback Method

Sources

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=C1768316&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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