

2-Propanone, 1,1,3-trichloro-

Other names:	«alpha», «alpha»', «alpha»'-Trichloroacetone 1,1,3-Trichloroacetone 1,1,3-Trichloro-2-propanone
Inchi:	InChI=1S/C3H3Cl3O/c4-1-2(7)3(5)6/h3H,1H2
InchiKey:	ZWILTCXCTVMANU-UHFFFAOYSA-N
Formula:	C3H3Cl3O
SMILES:	O=C(CCl)C(Cl)Cl
Mol. weight [g/mol]:	161.41
CAS:	921-03-9

Physical Properties

Property code	Value	Unit	Source
gf	-192.77	kJ/mol	Joback Method
hf	-270.33	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	41.78	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.598		Crippen Method
mcvol	91.420	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
rinpol	940.00		NIST Webbook
tb	445.20	K	NIST Webbook
tc	643.42	K	Joback Method
tf	248.26	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.64	J/molxK	433.76	Joback Method
cpg	142.73	J/molxK	468.70	Joback Method
cpg	147.52	J/molxK	503.65	Joback Method
cpg	152.00	J/molxK	538.59	Joback Method
cpg	156.20	J/molxK	573.53	Joback Method

cpg	160.13	J/molxK	608.48	Joback Method
cpg	163.78	J/molxK	643.42	Joback Method
dvisc	0.0048954	Paxs	248.26	Joback Method
dvisc	0.0026323	Paxs	279.18	Joback Method
dvisc	0.0016018	Paxs	310.09	Joback Method
dvisc	0.0010666	Paxs	341.01	Joback Method
dvisc	0.0007599	Paxs	371.93	Joback Method
dvisc	0.0005703	Paxs	402.84	Joback Method
dvisc	0.0004459	Paxs	433.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C921039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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