

2-Propanone, 1,1,3,3-tetrachloro-

Other names:	1,1,3,3-Tetrachloroacetone TCA 1,1,3,3-Tetrachloropropanone 1,1,3,3-Tetrachloro-2-propanone
Inchi:	InChI=1S/C3H2Cl4O/c4-2(5)1(8)3(6)7/h2-3H
InchiKey:	DJWVKJAGMVZYFP-UHFFFAOYSA-N
Formula:	C3H2Cl4O
SMILES:	O=C(C(Cl)Cl)C(Cl)Cl
Mol. weight [g/mol]:	195.86
CAS:	632-21-3

Physical Properties

Property code	Value	Unit	Source
gf	-207.14	kJ/mol	Joback Method
hf	-291.35	kJ/mol	Joback Method
hfus	14.87	kJ/mol	Joback Method
hvap	45.78	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.163		Crippen Method
mcvol	103.660	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	999.00		NIST Webbook
tb	470.75	K	Joback Method
tc	692.15	K	Joback Method
tf	263.18	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.87	J/molxK	470.75	Joback Method
cpg	160.73	J/molxK	507.65	Joback Method
cpg	165.24	J/molxK	544.55	Joback Method
cpg	169.40	J/molxK	581.45	Joback Method

cpg	173.23	J/molxK	618.35	Joback Method
cpg	176.75	J/molxK	655.25	Joback Method
cpg	179.98	J/molxK	692.15	Joback Method
dvisc	0.0062386	Paxs	263.18	Joback Method
dvisc	0.0030785	Paxs	297.77	Joback Method
dvisc	0.0017597	Paxs	332.37	Joback Method
dvisc	0.0011178	Paxs	366.97	Joback Method
dvisc	0.0007677	Paxs	401.56	Joback Method
dvisc	0.0005597	Paxs	436.15	Joback Method
dvisc	0.0004274	Paxs	470.75	Joback Method

Sources

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=C632213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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