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

Other names: «alpha»,«alpha»,«alpha»-Trichloroacetone
Trichloroacetone
1,1,1-Trichloroacetone
1,1,1-Trichloropropanone
1,1,1-Trichloro-2-propanone
CCl3COCH3
Inchi: InChI=1S/C3H3Cl3O/c1-2(7)3(4,5)6/h1H3
InchiKey: SMZHKGXSEAGRTI-UHFFFAOYSA-N
Formula: C3H3Cl3O
SMILES: CC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 161.41
CAS: 918-00-3

Physical Properties

Property code	Value	Unit	Source
affp	768.30	kJ/mol	NIST Webbook
basg	736.30	kJ/mol	NIST Webbook
gf	-187.49	kJ/mol	Joback Method
hf	-273.80	kJ/mol	Joback Method
hfus	10.30	kJ/mol	Joback Method
hvap	40.88	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.946		Crippen Method
mcvol	91.420	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	407.70	K	NIST Webbook
tc	650.04	K	Joback Method
tf	265.68	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.59	J/mol×K	430.97	Joback Method

cpg	146.38	J/mol×K	467.48	Joback Method
cpg	151.65	J/mol×K	503.99	Joback Method
cpg	156.44	J/mol×K	540.51	Joback Method
cpg	160.78	J/mol×K	577.02	Joback Method
cpg	164.71	J/mol×K	613.53	Joback Method
cpg	168.25	J/mol×K	650.04	Joback Method
dvisc	0.0048742	Pa×s	265.68	Joback Method
dvisc	0.0027744	Pa×s	293.23	Joback Method
dvisc	0.0017397	Pa×s	320.78	Joback Method
dvisc	0.0011745	Pa×s	348.33	Joback Method
dvisc	0.0008399	Pa×s	375.87	Joback Method
dvisc	0.0006287	Pa×s	403.42	Joback Method
dvisc	0.0004884	Pa×s	430.97	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=C918003&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume