2-Propanol, 1,1,1-trichloro-2-methyl-

Other names:	«beta»,«beta»,«beta»-Trichloro-tert-butyl alcohol
	Acetochlorone
	Acetone chloroform
	Chlorobutanol
	Chlorbutanol
	Chlorbutol
	Chloreton
	Chloretone
	Chlortran
	Clortran
	Dentalone
	Khloreton
	Methaform
	Sedaform
	Trichloro-tert-butyl alcohol
	1,1,1-Trichloro-tert-butyl alcohol
	2-(Trichloromethyl)-2-propanol
	2-(Trichloromethyl)propan-2-ol
	1,1,1-Trichloro-2-methyl-2-propanol
	tert-Trichlorobutyl alcohol
	Acetonchloroform
	HCP
	2-Propanol, 2-methyl-1,1,1-trichloro-
	Trichloro-tert-butanol
	Trichloro-t-butyl alcohol
	t-Trichlorobutyl alcohol
	2,2,2-Trichloro-1,1-dimethylethanol
	Coliquifilm
	Trichlorobutanol
	Anhydrous chlorobutanol
	NSC 44794
Inchi:	InChI=1S/C4H7Cl3O/c1-3(2,8)4(5,6)7/h8H,1-2H3
InchiKey:	OSASVXMJTNOKOY-UHFFFAOYSA-N
Formula:	C4H7Cl3O
SMILES:	CC(C)(O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	177.46
CAS:	57-15-8

Physical Properties

Property code	Value	Unit	Source
gf	-184.13	kJ/mol	Joback Method
hf	-342.84	kJ/mol	Joback Method
hfus	7.97	kJ/mol	Joback Method
hvap	51.74	kJ/mol	Joback Method
ie	10.38	eV	NIST Webbook
log10ws	-2.43		Crippen Method
logp	2.128		Crippen Method
mcvol	109.810	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	976.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1638.00		NIST Webbook
tb	440.20	K	NIST Webbook
tb	442.00 ± 4.00	K	NIST Webbook
tc	694.13	K	Joback Method
tf	371.90 ± 1.50	K	NIST Webbook
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.55	J/mol×K	488.93	Joback Method
cpg	237.95	J/mol×K	659.93	Joback Method
cpg	232.81	J/mol×K	625.73	Joback Method
cpg	227.15	J/mol×K	591.53	Joback Method
cpg	220.93	J/mol×K	557.33	Joback Method
cpg	214.08	J/mol×K	523.13	Joback Method
cpg	242.62	J/mol×K	694.13	Joback Method
dvisc	0.0002274	Pa×s	488.93	Joback Method
dvisc	0.0003769	Pa×s	455.82	Joback Method
dvisc	0.0006763	Pa×s	422.71	Joback Method
dvisc	0.0013403	Pa×s	389.60	Joback Method

dvisc	0.0030159	Pa×s	356.48	Joback Method
dvisc	0.0080124	Pa×s	323.37	Joback Method
dvisc	0.0266028	Pa×s	290.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57158&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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume