Ethanol, 2,2,2-trichloro-

Other names:	«beta»,«beta»,.beta-Trichloroethanol
	(Hydroxymethyl)trichloromethane
	Trichlorethanol
	Trichloroethanol
	2,2,2-Trichloroethanol
	2,2,2-Trichloroethyl alcohol
	CCl3CH2OH
	Trichloroethyl alcohol
	2,2,2-Trichloro-1-ethanol
	NSC 66407
Inchi:	InChI=1S/C2H3Cl3O/c3-2(4,5)1-6/h6H,1H2
InchiKey:	KPWDGTGXUYRARH-UHFFFAOYSA-N
Formula:	C2H3Cl3O
SMILES:	OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	149.40
CAS:	115-20-8

Physical Properties

Property code	Value	Unit	Source
affp	729.30	kJ/mol	NIST Webbook
basg	698.90	kJ/mol	NIST Webbook
gf	-203.81	kJ/mol	Joback Method
hf	-292.81	kJ/mol	Joback Method
hfus	10.20	kJ/mol	Joback Method
hvap	48.58	kJ/mol	Joback Method
ie	10.94	eV	NIST Webbook
ie	13.60	eV	NIST Webbook
log10ws	-1.48		Crippen Method
logp	1.349		Crippen Method
mcvol	81.630	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
rinpol	838.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	857.00		NIST Webbook

rinpol	859.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	858.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1701.00		NIST Webbook
tb	424.20	K	NIST Webbook
tb	424.00 ± 1.00	K	NIST Webbook
tc	643.79	K	Joback Method
tf	265.30	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.30	J/mol×K	643.79	Joback Method
cpg	128.88	J/mol×K	446.40	Joback Method
cpg	133.14	J/mol×K	479.30	Joback Method
cpg	137.02	J/mol×K	512.20	Joback Method
cpg	140.55	J/mol×K	545.09	Joback Method
cpg	143.76	J/mol×K	577.99	Joback Method
cpg	146.67	J/mol×K	610.89	Joback Method
dvisc	0.0003610	Pa×s	446.40	Joback Method
dvisc	0.0340226	Pa×s	265.30	Joback Method
dvisc	0.0108307	Pa×s	295.48	Joback Method
dvisc	0.0042628	Pa×s	325.67	Joback Method
dvisc	0.0019653	Pa×s	355.85	Joback Method
dvisc	0.0010227	Pa×s	386.03	Joback Method
dvisc	0.0005851	Pa×s	416.22	Joback Method
hfust	10.05	kJ/mol	290.60	NIST Webbook

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=C115208&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
hfust:	Enthalpy of fusion at a given temperature
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