Ethanol, 2-chloro, trichloroacetate

Other names: Ethanol, 2-chloro, trichloroacetate
Inchi: InChI=1S/C4H4Cl4O2/c5-1-2-10-3(9)4(6,7)8/h1-2H2
InchiKey: LZAFIYKPGDSKLN-UHFFFAOYSA-N
Formula: C4H4Cl4O2
SMILES: O=C(OCCCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 225.89

Physical Properties

Property code	Value	Unit	Source
hf	-452.46	kJ/mol	Cheméo Relay (1.0)
hfus	18.28	kJ/mol	Joback Method
hvap	56.40	kJ/mol	Cheméo Relay (1.0)
logp	2.139		Crippen Method
mcvol	123.620	ml/mol	McGowan Method
rinpol	1139.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1152.00		NIST Webbook
ripol	1873.00		NIST Webbook
ripol	1859.00		NIST Webbook
ripol	1852.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1849.00		NIST Webbook
tb	478.48	K	Cheméo Relay (1.0)
tf	272.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.23	J/mol×K	513.70	Joback Method
cpg	221.68	J/mol×K	550.32	Joback Method
cpg	227.63	J/mol×K	586.95	Joback Method
cpg	233.12	J/mol×K	623.57	Joback Method
cpg	238.15	J/mol×K	660.20	Joback Method

cpg	242.76	J/mol×K	696.82	Joback Method
cpg	246.97	J/mol×K	733.45	Joback Method
dvisc	0.0028944	Pa×s	329.10	Joback Method
dvisc	0.0017300	Pa×s	359.87	Joback Method
dvisc	0.0011213	Pa×s	390.63	Joback Method
dvisc	0.0007743	Pa×s	421.40	Joback Method
dvisc	0.0005623	Pa×s	452.17	Joback Method
dvisc	0.0004254	Pa×s	482.93	Joback Method
dvisc	0.0003327	Pa×s	513.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4974214&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point