Ethanol, 2-chloro, chloroacetate

Other names: Ethanol, 2-chloro, chloroacetate
Inchi: InChI=1S/C4H6Cl2O2/c5-1-2-8-4(7)3-6/h1-3H2
InchiKey: XPUCYTFPMSEFIN-UHFFFAOYSA-N
Formula: C4H6Cl2O2
SMILES: O=C(CCl)OCCCl
Mol. weight [g/mol]: 157.00

Physical Properties

Property code	Value	Unit	Source
hf	-471.58	kJ/mol	Cheméo Relay (1.0)
hfus	17.30	kJ/mol	Joback Method
hvap	47.08	kJ/mol	Cheméo Relay (1.0)
ie	10.64	eV	Cheméo Relay (1.0)
logp	1.007		Crippen Method
mcvol	99.140	ml/mol	McGowan Method
rinpol	990.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1002.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1755.00		NIST Webbook
tb	462.15	K	Cheméo Relay (1.0)
tf	261.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.53	J/mol×K	604.27	Joback Method
cpg	207.89	J/mol×K	636.71	Joback Method
cpg	178.56	J/mol×K	474.51	Joback Method

cpg	184.93	J/mol×K	506.95	Joback Method
cpg	191.05	J/mol×K	539.39	Joback Method
cpg	196.92	J/mol×K	571.83	Joback Method
cpg	171.94	J/mol×K	442.07	Joback Method
dvisc	0.0011043	Pa×s	325.25	Joback Method
dvisc	0.0016875	Pa×s	296.05	Joback Method
dvisc	0.0028294	Pa×s	266.84	Joback Method
dvisc	0.0007750	Pa×s	354.46	Joback Method
dvisc	0.0005740	Pa×s	383.66	Joback Method
dvisc	0.0004436	Pa×s	412.87	Joback Method
dvisc	0.0003546	Pa×s	442.07	Joback Method
hvapt	53.30	kJ/mol	398.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C3848122&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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