2,2,2-Trichloroethyl acetate

Other names: Acetic acid, 2,2,2-trichloroethyl ester
Inchi: InChI=1S/C4H5Cl3O2/c1-3(8)9-2-4(5,6)7/h2H2,1H3
InchiKey: XHAXVDWUMCHTCY-UHFFFAOYSA-N
Formula: C4H5Cl3O2
SMILES: CC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 191.44
CAS: 625-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-284.07	kJ/mol	Joback Method
hf	-426.66	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	45.51	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.920		Crippen Method
mcvol	111.380	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	974.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	988.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1422.00		NIST Webbook
tb	476.27	K	Joback Method
tc	690.53	K	Joback Method
tf	299.18	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.64	J/mol×K	476.27	Joback Method
cpg	202.69	J/mol×K	511.98	Joback Method
cpg	209.27	J/mol×K	547.69	Joback Method
cpg	215.39	J/mol×K	583.40	Joback Method
cpg	221.07	J/mol×K	619.11	Joback Method
cpg	226.33	J/mol×K	654.82	Joback Method
cpg	231.19	J/mol×K	690.53	Joback Method
dvisc	0.0033897	Pa×s	299.18	Joback Method
dvisc	0.0019690	Pa×s	328.69	Joback Method
dvisc	0.0012509	Pa×s	358.21	Joback Method
dvisc	0.0008515	Pa×s	387.73	Joback Method
dvisc	0.0006120	Pa×s	417.24	Joback Method
dvisc	0.0004595	Pa×s	446.75	Joback Method
dvisc	0.0003575	Pa×s	476.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625241&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

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