3-chloropropyl trichloroacetate

Other names: 1-Propanol, 3-chloro, trichloroacetate
Inchi: InChI=1S/C5H6Cl4O2/c6-2-1-3-11-4(10)5(7,8)9/h1-3H2
InchiKey: SUOYAKIYUAIFGY-UHFFFAOYSA-N
Formula: C5H6Cl4O2
SMILES: O=C(OCCCCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 239.91

Physical Properties

Property code	Value	Unit	Source
gf	-287.58	kJ/mol	Joback Method
hf	-463.04	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	52.12	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.529		Crippen Method
mcvol	137.710	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1251.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1944.00		NIST Webbook
ripol	1931.00		NIST Webbook
ripol	1921.00		NIST Webbook
ripol	1895.00		NIST Webbook
tb	536.58	K	Joback Method
tc	752.64	K	Joback Method
tf	340.37	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.56	J/mol×K	536.58	Joback Method
cpg	263.24	J/mol×K	572.59	Joback Method
cpg	270.37	J/mol×K	608.60	Joback Method
cpg	276.98	J/mol×K	644.61	Joback Method
cpg	283.08	J/mol×K	680.62	Joback Method
cpg	288.70	J/mol×K	716.63	Joback Method
cpg	293.88	J/mol×K	752.64	Joback Method
dvisc	0.0027219	Pa×s	340.37	Joback Method
dvisc	0.0015950	Pa×s	373.07	Joback Method
dvisc	0.0010187	Pa×s	405.77	Joback Method
dvisc	0.0006957	Pa×s	438.48	Joback Method
dvisc	0.0005009	Pa×s	471.18	Joback Method
dvisc	0.0003763	Pa×s	503.88	Joback Method
dvisc	0.0002928	Pa×s	536.58	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112595&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