5-chloropentyl trichloroacetate

Other names: 1-Pentanol, 5-chloro, trichloroacetate
Inchi: InChI=1S/C7H10Cl4O2/c8-4-2-1-3-5-13-6(12)7(9,10)11/h1-5H2
InchiKey: RNDGFCISXTXPID-UHFFFAOYSA-N
Formula: C7H10Cl4O2
SMILES: O=C(OCCCCCCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 267.96

Physical Properties

Property code	Value	Unit	Source
gf	-270.74	kJ/mol	Joback Method
hf	-504.32	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	56.58	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.309		Crippen Method
mcvol	165.890	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1523.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1513.00		NIST Webbook
ripol	2155.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2188.00		NIST Webbook
ripol	2205.00		NIST Webbook
tb	582.34	K	Joback Method
tc	791.37	K	Joback Method
tf	362.91	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.86	J/mol×K	582.34	Joback Method

cpg	384.37	J/mol×K	756.53	Joback Method
cpg	377.04	J/mol×K	721.69	Joback Method
cpg	369.15	J/mol×K	686.85	Joback Method
cpg	360.68	J/mol×K	652.02	Joback Method
cpg	351.59	J/mol×K	617.18	Joback Method
cpg	391.17	J/mol×K	791.37	Joback Method
dvisc	0.0002240	Pa×s	582.34	Joback Method
dvisc	0.0002906	Pa×s	545.77	Joback Method
dvisc	0.0003915	Pa×s	509.20	Joback Method
dvisc	0.0005522	Pa×s	472.62	Joback Method
dvisc	0.0008252	Pa×s	436.05	Joback Method
dvisc	0.0013273	Pa×s	399.48	Joback Method
dvisc	0.0023494	Pa×s	362.91	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112486&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