2-chloropentyl trichloroacetate

Other names: 1-Pentanol, 2-chloro, trichloroacetate
Inchi: InChI=1S/C7H10Cl4O2/c1-2-3-5(8)4-13-6(12)7(9,10)11/h5H,2-4H2,1H3
InchiKey: KLZWAXURZZRALT-UHFFFAOYSA-N
Formula: C7H10Cl4O2
SMILES: CCCC(Cl)COC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 267.96

Physical Properties

Property code	Value	Unit	Source
gf	-273.18	kJ/mol	Joback Method
hf	-509.60	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	56.19	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.307		Crippen Method
mcvol	165.890	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1387.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1393.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1935.00		NIST Webbook
ripol	1908.00		NIST Webbook
ripol	1905.00		NIST Webbook
tb	581.90	K	Joback Method
tc	795.32	K	Joback Method
tf	347.91	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.31	J/mol×K	581.90	Joback Method

cpg	385.77	J/mol×K	759.75	Joback Method
cpg	378.32	J/mol×K	724.18	Joback Method
cpg	370.28	J/mol×K	688.61	Joback Method
cpg	361.62	J/mol×K	653.04	Joback Method
cpg	352.30	J/mol×K	617.47	Joback Method
cpg	392.66	J/mol×K	795.32	Joback Method
dvisc	0.0002097	Pa×s	581.90	Joback Method
dvisc	0.0002785	Pa×s	542.90	Joback Method
dvisc	0.0003867	Pa×s	503.90	Joback Method
dvisc	0.0005673	Pa×s	464.90	Joback Method
dvisc	0.0008926	Pa×s	425.91	Joback Method
dvisc	0.0015388	Pa×s	386.91	Joback Method
dvisc	0.0029975	Pa×s	347.91	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112397&Units=SI

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