5-chlorooctyl trichloroacetate

Other names: 1-Octanol, 5-chloro, trichloroacetate
Inchi: InChI=1S/C10H16Cl4O2/c1-2-5-8(11)6-3-4-7-16-9(15)10(12,13)14/h8H,2-7H2,1H3
InchiKey: WMIQRQVSKHSOFB-UHFFFAOYSA-N
Formula: C10H16Cl4O2
SMILES: CCCC(Cl)CCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 310.05

Physical Properties

Property code	Value	Unit	Source
gf	-247.92	kJ/mol	Joback Method
hf	-571.52	kJ/mol	Joback Method
hfus	30.29	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.478		Crippen Method
mcvol	208.160	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1770.00		NIST Webbook
ripol	2338.00		NIST Webbook
ripol	2315.00		NIST Webbook
ripol	2355.00		NIST Webbook
tb	650.54	K	Joback Method
tc	854.25	K	Joback Method
tf	381.72	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.42	J/mol×K	650.54	Joback Method
cpg	538.14	J/mol×K	820.30	Joback Method

cpg	528.80	J/mol×K	786.35	Joback Method
cpg	518.80	J/mol×K	752.39	Joback Method
cpg	508.09	J/mol×K	718.44	Joback Method
cpg	496.64	J/mol×K	684.49	Joback Method
cpg	546.84	J/mol×K	854.25	Joback Method
dvisc	0.0001358	Pa×s	650.54	Joback Method
dvisc	0.0001822	Pa×s	605.74	Joback Method
dvisc	0.0002562	Pa×s	560.93	Joback Method
dvisc	0.0003821	Pa×s	516.13	Joback Method
dvisc	0.0006150	Pa×s	471.33	Joback Method
dvisc	0.0010938	Pa×s	426.52	Joback Method
dvisc	0.0022272	Pa×s	381.72	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=R112228&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