7-chlorooctyl dichloroacetate

Other names: 1-Octanol, 7-chloro, dichloroacetate
Inchi: InChI=1S/C10H17Cl3O2/c1-8(11)6-4-2-3-5-7-15-10(14)9(12)13/h8-9H,2-7H2,1H3
InchiKey: WMRINDHNJPJHEX-UHFFFAOYSA-N
Formula: C10H17Cl3O2
SMILES: CC(Cl)CCCCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 275.60

Physical Properties

Property code	Value	Unit	Source
gf	-241.27	kJ/mol	Joback Method
hf	-552.31	kJ/mol	Joback Method
hfus	29.99	kJ/mol	Joback Method
hvap	59.39	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.911		Crippen Method
mcvol	195.920	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1682.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1682.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2416.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2404.00		NIST Webbook
tb	615.90	K	Joback Method
tc	809.16	K	Joback Method
tf	334.38	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	455.66	J/mol×K	615.90	Joback Method
cpg	468.53	J/mol×K	648.11	Joback Method
cpg	480.73	J/mol×K	680.32	Joback Method
cpg	492.28	J/mol×K	712.53	Joback Method
cpg	503.19	J/mol×K	744.74	Joback Method
cpg	513.48	J/mol×K	776.95	Joback Method
cpg	523.15	J/mol×K	809.16	Joback Method
dvisc	0.0033761	Pa×s	334.38	Joback Method
dvisc	0.0014970	Pa×s	381.30	Joback Method
dvisc	0.0007933	Pa×s	428.22	Joback Method
dvisc	0.0004765	Pa×s	475.14	Joback Method
dvisc	0.0003137	Pa×s	522.06	Joback Method
dvisc	0.0002213	Pa×s	568.98	Joback Method
dvisc	0.0001646	Pa×s	615.90	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112273&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