3-chlorooctyl dichloroacetate

Other names: 1-Octanol, 3-chloro, dichloroacetate
Inchi: InChI=1S/C10H17Cl3O2/c1-2-3-4-5-8(11)6-7-15-10(14)9(12)13/h8-9H,2-7H2,1H3
InchiKey: VLFLWPGLPMXFEF-UHFFFAOYSA-N
Formula: C10H17Cl3O2
SMILES: CCCCCC(Cl)CCOC(=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	1645.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1637.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2291.00		NIST Webbook
ripol	2281.00		NIST Webbook
ripol	2266.00		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	513.48	J/mol×K	776.95	Joback Method
cpg	503.19	J/mol×K	744.74	Joback Method
cpg	492.28	J/mol×K	712.53	Joback Method
cpg	480.73	J/mol×K	680.32	Joback Method
cpg	468.53	J/mol×K	648.11	Joback Method
cpg	523.15	J/mol×K	809.16	Joback Method
dvisc	0.0001646	Pa×s	615.90	Joback Method
dvisc	0.0002213	Pa×s	568.98	Joback Method
dvisc	0.0003137	Pa×s	522.06	Joback Method
dvisc	0.0004765	Pa×s	475.14	Joback Method
dvisc	0.0007933	Pa×s	428.22	Joback Method
dvisc	0.0014970	Pa×s	381.30	Joback Method
dvisc	0.0033761	Pa×s	334.38	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=R112159&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