8-chlorooctyl dichloroacetate

Other names: 1-Octanol, 8-chloro, dichloroacetate
Inchi: InChI=1S/C10H17Cl3O2/c11-7-5-3-1-2-4-6-8-15-10(14)9(12)13/h9H,1-8H2
InchiKey: FDJHTHGSNGTWSO-UHFFFAOYSA-N
Formula: C10H17Cl3O2
SMILES: O=C(OCCCCCCCCCl)C(Cl)Cl
Mol. weight [g/mol]: 275.60

Physical Properties

Property code	Value	Unit	Source
gf	-238.83	kJ/mol	Joback Method
hf	-547.03	kJ/mol	Joback Method
hfus	33.51	kJ/mol	Joback Method
hvap	59.78	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.913		Crippen Method
mcvol	195.920	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1761.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1736.00		NIST Webbook
ripol	2491.00		NIST Webbook
ripol	2470.00		NIST Webbook
ripol	2470.00		NIST Webbook
ripol	2506.00		NIST Webbook
tb	616.34	K	Joback Method
tc	806.15	K	Joback Method
tf	349.38	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	455.20	J/mol×K	616.34	Joback Method
cpg	467.80	J/mol×K	647.97	Joback Method
cpg	479.77	J/mol×K	679.61	Joback Method
cpg	491.10	J/mol×K	711.24	Joback Method
cpg	501.83	J/mol×K	742.88	Joback Method
cpg	511.97	J/mol×K	774.51	Joback Method
cpg	521.52	J/mol×K	806.15	Joback Method
dvisc	0.0026084	Pa×s	349.38	Joback Method
dvisc	0.0012923	Pa×s	393.87	Joback Method
dvisc	0.0007384	Pa×s	438.37	Joback Method
dvisc	0.0004677	Pa×s	482.86	Joback Method
dvisc	0.0003200	Pa×s	527.35	Joback Method
dvisc	0.0002323	Pa×s	571.85	Joback Method
dvisc	0.0001766	Pa×s	616.34	Joback Method

Sources

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=R112302&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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