Dichloroacetic acid, hexyl ester

Other names:	1-Hexanol, dichloroacetate
	Hexyl dichloroacetate
Inchi:	InChI=1S/C8H14Cl2O2/c1-2-3-4-5-6-12-8(11)7(9)10/h7H,2-6H2,1H3
InchiKey:	WZSTYEOGVNOGKU-UHFFFAOYSA-N
Formula:	C8H14Cl2O2
SMILES:	CCCCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]:	213.10
CAS:	37079-04-2

Physical Properties

Property code	Value	Unit	Source
gf	-243.74	kJ/mol	Joback Method
hf	-490.01	kJ/mol	Joback Method
hfus	24.13	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.914		Crippen Method
mcvol	155.500	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1278.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1285.50		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1270.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1759.00		NIST Webbook
tb	533.15	K	Joback Method
tc	722.96	K	Joback Method
tf	296.92	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.71	J/mol×K	533.15	Joback Method
cpg	346.37	J/mol×K	564.79	Joback Method
cpg	357.50	J/mol×K	596.42	Joback Method
cpg	368.12	J/mol×K	628.06	Joback Method
cpg	378.23	J/mol×K	659.69	Joback Method
cpg	387.84	J/mol×K	691.33	Joback Method
cpg	396.95	J/mol×K	722.96	Joback Method
dvisc	0.0035993	Pa×s	296.92	Joback Method
dvisc	0.0017614	Pa×s	336.29	Joback Method
dvisc	0.0010012	Pa×s	375.66	Joback Method
dvisc	0.0006335	Pa×s	415.03	Joback Method
dvisc	0.0004339	Pa×s	454.41	Joback Method
dvisc	0.0003157	Pa×s	493.78	Joback Method
dvisc	0.0002408	Pa×s	533.15	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37079042&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