6-chlorohexyl dichloroacetate

Other names: 1-Hexanol, 6-chloro, dichloroacetate
Inchi: InChI=1S/C8H13Cl3O2/c9-5-3-1-2-4-6-13-8(12)7(10)11/h7H,1-6H2
InchiKey: NTHUGYDCPBABME-UHFFFAOYSA-N
Formula: C8H13Cl3O2
SMILES: O=C(OCCCCCCCl)C(Cl)Cl
Mol. weight [g/mol]: 247.55

Physical Properties

Property code	Value	Unit	Source
gf	-255.67	kJ/mol	Joback Method
hf	-505.75	kJ/mol	Joback Method
hfus	28.33	kJ/mol	Joback Method
hvap	55.33	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.133		Crippen Method
mcvol	167.740	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1509.00		NIST Webbook
ripol	2281.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2281.00		NIST Webbook
tb	570.58	K	Joback Method
tc	765.02	K	Joback Method
tf	326.84	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.24	J/mol×K	570.58	Joback Method
cpg	410.08	J/mol×K	732.61	Joback Method
cpg	401.17	J/mol×K	700.21	Joback Method
cpg	391.74	J/mol×K	667.80	Joback Method
cpg	381.78	J/mol×K	635.39	Joback Method
cpg	371.28	J/mol×K	602.99	Joback Method
cpg	418.47	J/mol×K	765.02	Joback Method
dvisc	0.0002252	Pa×s	570.58	Joback Method
dvisc	0.0002939	Pa×s	529.96	Joback Method
dvisc	0.0004011	Pa×s	489.33	Joback Method
dvisc	0.0005789	Pa×s	448.71	Joback Method
dvisc	0.0008990	Pa×s	408.09	Joback Method
dvisc	0.0015387	Pa×s	367.46	Joback Method
dvisc	0.0030100	Pa×s	326.84	Joback Method

Sources

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=R112040&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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