2-chlorohexyl dichloroacetate

Other names: 1-Hexanol, 2-chloro, dichloroacetate
Inchi: InChI=1S/C8H13Cl3O2/c1-2-3-4-6(9)5-13-8(12)7(10)11/h6-7H,2-5H2,1H3
InchiKey: PFUJZHGZRURGIP-UHFFFAOYSA-N
Formula: C8H13Cl3O2
SMILES: CCCCC(Cl)COC(=O)C(Cl)Cl
Mol. weight [g/mol]: 247.55

Physical Properties

Property code	Value	Unit	Source
gf	-258.11	kJ/mol	Joback Method
hf	-511.03	kJ/mol	Joback Method
hfus	24.81	kJ/mol	Joback Method
hvap	54.94	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.131		Crippen Method
mcvol	167.740	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1396.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1396.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2047.00		NIST Webbook
tb	570.14	K	Joback Method
tc	768.49	K	Joback Method
tf	311.84	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	360.64	J/mol×K	570.14	Joback Method
cpg	371.97	J/mol×K	603.20	Joback Method
cpg	382.72	J/mol×K	636.26	Joback Method
cpg	392.89	J/mol×K	669.32	Joback Method
cpg	402.51	J/mol×K	702.37	Joback Method
cpg	411.57	J/mol×K	735.43	Joback Method
cpg	420.09	J/mol×K	768.49	Joback Method
dvisc	0.0039796	Pa×s	311.84	Joback Method
dvisc	0.0018126	Pa×s	354.89	Joback Method
dvisc	0.0009788	Pa×s	397.94	Joback Method
dvisc	0.0005961	Pa×s	440.99	Joback Method
dvisc	0.0003965	Pa×s	484.04	Joback Method
dvisc	0.0002819	Pa×s	527.09	Joback Method
dvisc	0.0002110	Pa×s	570.14	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=R111923&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

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