

3-chlorohexyl dichloroacetate

Other names:	1-Hexanol, 3-chloro, dichloroacetate
Inchi:	InChI=1S/C8H13Cl3O2/c1-2-3-6(9)4-5-13-8(12)7(10)11/h6-7H,2-5H2,1H3
InchiKey:	RIDFFRLCBOOJKN-UHFFFAOYSA-N
Formula:	C8H13Cl3O2
SMILES:	CCCC(CI)CCOC(=O)C(CI)CI
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	1433.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1451.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2085.00		NIST Webbook
tb	570.14	K	Joback Method
tc	768.49	K	Joback Method
tf	311.84	K	Joback Method
vc	0.642	m ³ /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/molxK	603.20	Joback Method
cpg	382.72	J/molxK	636.26	Joback Method
cpg	392.89	J/molxK	669.32	Joback Method
cpg	402.51	J/molxK	702.37	Joback Method
cpg	411.57	J/molxK	735.43	Joback Method
cpg	420.09	J/molxK	768.49	Joback Method
dvisc	0.0039796	Paxs	311.84	Joback Method
dvisc	0.0018126	Paxs	354.89	Joback Method
dvisc	0.0009788	Paxs	397.94	Joback Method
dvisc	0.0005961	Paxs	440.99	Joback Method
dvisc	0.0003965	Paxs	484.04	Joback Method
dvisc	0.0002819	Paxs	527.09	Joback Method
dvisc	0.0002110	Paxs	570.14	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=R111958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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