

5-chloroheptyl dichloroacetate

Other names:	1-Heptanol, 5-chloro, dichloroacetate
Inchi:	InChI=1S/C9H15Cl3O2/c1-2-7(10)5-3-4-6-14-9(13)8(11)12/h7-8H,2-6H2,1H3
InchiKey:	TUHGJLNONAKZDJ-UHFFFAOYSA-N
Formula:	C9H15Cl3O2
SMILES:	CCC(Cl)CCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]:	261.57

Physical Properties

Property code	Value	Unit	Source
gf	-249.69	kJ/mol	Joback Method
hf	-531.67	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.521		Crippen Method
mcvol	181.830	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1599.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1586.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2290.00		NIST Webbook
ripol	2300.00		NIST Webbook
tb	593.02	K	Joback Method
tc	788.71	K	Joback Method
tf	323.11	K	Joback Method
vc	0.699	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.32	J/mol×K	593.02	Joback Method

cpg	419.47	J/molxK	625.64	Joback Method
cpg	431.00	J/molxK	658.25	Joback Method
cpg	441.90	J/molxK	690.87	Joback Method
cpg	452.21	J/molxK	723.48	Joback Method
cpg	461.92	J/molxK	756.10	Joback Method
cpg	471.06	J/molxK	788.71	Joback Method
dvisc	0.0036788	Paxs	323.11	Joback Method
dvisc	0.0016526	Paxs	368.10	Joback Method
dvisc	0.0008837	Paxs	413.08	Joback Method
dvisc	0.0005344	Paxs	458.06	Joback Method
dvisc	0.0003536	Paxs	503.05	Joback Method
dvisc	0.0002504	Paxs	548.03	Joback Method
dvisc	0.0001868	Paxs	593.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111785&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

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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