3-chloroheptyl dichloroacetate

Other names: 1-Heptanol, 3-chloro, dichloroacetate
Inchi: InChI=1S/C9H15Cl3O2/c1-2-3-4-7(10)5-6-14-9(13)8(11)12/h7-8H,2-6H2,1H3
InchiKey: XNURRQZRWQLOON-UHFFFAOYSA-N
Formula: C9H15Cl3O2
SMILES: CCCCC(Cl)CCOC(=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	1537.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1527.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2196.00		NIST Webbook
ripol	2188.00		NIST Webbook
tb	593.02	K	Joback Method
tc	788.71	K	Joback Method
tf	323.11	K	Joback Method
vc	0.699	m3/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/mol×K	625.64	Joback Method

cpg	431.00	J/mol×K	658.25	Joback Method
cpg	441.90	J/mol×K	690.87	Joback Method
cpg	452.21	J/mol×K	723.48	Joback Method
cpg	461.92	J/mol×K	756.10	Joback Method
cpg	471.06	J/mol×K	788.71	Joback Method
dvisc	0.0036788	Pa×s	323.11	Joback Method
dvisc	0.0016526	Pa×s	368.10	Joback Method
dvisc	0.0008837	Pa×s	413.08	Joback Method
dvisc	0.0005344	Pa×s	458.06	Joback Method
dvisc	0.0003536	Pa×s	503.05	Joback Method
dvisc	0.0002504	Pa×s	548.03	Joback Method
dvisc	0.0001868	Pa×s	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=R111725&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