(E)-3-Hexen-1-ol, dichloroacetate

Inchi: InChI=1S/C8H12Cl2O2/c1-2-3-4-5-6-12-8(11)7(9)10/h3-4,7H,2,5-6H2,1H3/b4-3+
InchiKey: RKUQPBWHNGASBI-ONEGZZNKSA-N
Formula: C8H12Cl2O2
SMILES: CCC=CCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 211.09

Physical Properties

Property code	Value	Unit	Source
gf	-163.52	kJ/mol	Joback Method
hf	-372.79	kJ/mol	Joback Method
hfus	24.34	kJ/mol	Joback Method
hvap	50.90	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.690		Crippen Method
mcvol	151.200	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1256.00		NIST Webbook
ripol	1751.00		NIST Webbook
tb	537.31	K	Joback Method
tc	735.49	K	Joback Method
tf	291.84	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.99	J/mol×K	537.31	Joback Method
cpg	327.12	J/mol×K	570.34	Joback Method
cpg	337.67	J/mol×K	603.37	Joback Method
cpg	347.66	J/mol×K	636.40	Joback Method
cpg	357.11	J/mol×K	669.43	Joback Method
cpg	366.05	J/mol×K	702.46	Joback Method
cpg	374.48	J/mol×K	735.49	Joback Method
dvisc	0.0033537	Pa×s	291.84	Joback Method

dvisc	0.0015786	Pa×s	332.75	Joback Method
dvisc	0.0008763	Pa×s	373.66	Joback Method
dvisc	0.0005464	Pa×s	414.57	Joback Method
dvisc	0.0003708	Pa×s	455.49	Joback Method
dvisc	0.0002683	Pa×s	496.40	Joback Method
dvisc	0.0002039	Pa×s	537.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26653&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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