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

Inchi: InChI=1S/C8H11Cl3O2/c1-2-3-4-5-6-13-7(12)8(9,10)11/h3-4H,2,5-6H2,1H3/b4-3+
InchiKey: HIHSJHFAKCBBNH-ONEGZZNKSA-N
Formula: C8H11Cl3O2
SMILES: CCC=CCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 245.53

Physical Properties

Property code	Value	Unit	Source
gf	-170.17	kJ/mol	Joback Method
hf	-392.00	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	54.38	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.256		Crippen Method
mcvol	163.440	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
ripol	1721.00		NIST Webbook
tb	571.95	K	Joback Method
tc	782.40	K	Joback Method
tf	339.18	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.62	J/mol×K	571.95	Joback Method
cpg	354.38	J/mol×K	607.03	Joback Method
cpg	364.41	J/mol×K	642.10	Joback Method
cpg	373.76	J/mol×K	677.18	Joback Method
cpg	382.47	J/mol×K	712.25	Joback Method
cpg	390.58	J/mol×K	747.33	Joback Method
cpg	398.14	J/mol×K	782.40	Joback Method

dvisc	0.0024957	Pa×s	339.18	Joback Method
dvisc	0.0012971	Pa×s	377.98	Joback Method
dvisc	0.0007615	Pa×s	416.77	Joback Method
dvisc	0.0004895	Pa×s	455.57	Joback Method
dvisc	0.0003372	Pa×s	494.36	Joback Method
dvisc	0.0002453	Pa×s	533.15	Joback Method
dvisc	0.0001863	Pa×s	571.95	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=R26671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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