4-Penten-1-ol, dichloroacetate

Inchi: InChI=1S/C7H10Cl2O2/c1-2-3-4-5-11-7(10)6(8)9/h2,6H,1,3-5H2
InchiKey: KWMRRMPMLGGEDX-UHFFFAOYSA-N
Formula: C7H10Cl2O2
SMILES: C=CCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 197.06

Physical Properties

Property code	Value	Unit	Source
gf	-164.32	kJ/mol	Joback Method
hf	-343.94	kJ/mol	Joback Method
hfus	20.26	kJ/mol	Joback Method
hvap	48.04	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.299		Crippen Method
mcvol	137.110	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1147.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1672.00		NIST Webbook
tb	506.95	K	Joback Method
tc	703.04	K	Joback Method
tf	283.89	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.07	J/mol×K	506.95	Joback Method
cpg	318.15	J/mol×K	670.36	Joback Method
cpg	310.06	J/mol×K	637.68	Joback Method
cpg	301.51	J/mol×K	605.00	Joback Method
cpg	292.50	J/mol×K	572.31	Joback Method
cpg	283.03	J/mol×K	539.63	Joback Method
cpg	325.80	J/mol×K	703.04	Joback Method

dvisc	0.0002712	Pa×s	506.95	Joback Method
dvisc	0.0003511	Pa×s	469.77	Joback Method
dvisc	0.0004751	Pa×s	432.60	Joback Method
dvisc	0.0006804	Pa×s	395.42	Joback Method
dvisc	0.0010501	Pa×s	358.24	Joback Method
dvisc	0.0017917	Pa×s	321.07	Joback Method
dvisc	0.0035164	Pa×s	283.89	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=R26493&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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