4-Penten-2-ol, dichloroacetate

Inchi: InChI=1S/C7H10Cl2O2/c1-3-4-5(2)11-7(10)6(8)9/h3,5-6H,1,4H2,2H3
InchiKey: USCBFFDOXIGWRO-UHFFFAOYSA-N
Formula: C7H10Cl2O2
SMILES: C=CCC(C)OC(=O)C(Cl)Cl
Mol. weight [g/mol]: 197.06

Physical Properties

Property code	Value	Unit	Source
gf	-166.76	kJ/mol	Joback Method
hf	-349.22	kJ/mol	Joback Method
hfus	16.74	kJ/mol	Joback Method
hvap	47.66	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.298		Crippen Method
mcvol	137.110	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1077.00		NIST Webbook
ripol	1548.00		NIST Webbook
ripol	1548.00		NIST Webbook
tb	506.51	K	Joback Method
tc	706.92	K	Joback Method
tf	268.89	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.36	J/mol×K	506.51	Joback Method
cpg	283.61	J/mol×K	539.91	Joback Method
cpg	293.35	J/mol×K	573.31	Joback Method
cpg	302.59	J/mol×K	606.71	Joback Method
cpg	311.34	J/mol×K	640.11	Joback Method
cpg	319.61	J/mol×K	673.51	Joback Method
cpg	327.41	J/mol×K	706.92	Joback Method

dvisc	0.0048985	Pa×s	268.89	Joback Method
dvisc	0.0021850	Pa×s	308.49	Joback Method
dvisc	0.0011712	Pa×s	348.10	Joback Method
dvisc	0.0007130	Pa×s	387.70	Joback Method
dvisc	0.0004759	Pa×s	427.30	Joback Method
dvisc	0.0003402	Pa×s	466.91	Joback Method
dvisc	0.0002563	Pa×s	506.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26564&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.