4-Penten-2-ol, chloroacetate

Inchi: InChI=1S/C7H11ClO2/c1-3-4-6(2)10-7(9)5-8/h3,6H,1,4-5H2,2H3
InchiKey: MLUZZPKUPKESMI-UHFFFAOYSA-N
Formula: C7H11ClO2
SMILES: C=CCC(C)OC(=O)CCl
Mol. weight [g/mol]: 162.61

Physical Properties

Property code	Value	Unit	Source
gf	-152.39	kJ/mol	Joback Method
hf	-328.20	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	43.66	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.733		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1004.00		NIST Webbook
ripol	1482.00		NIST Webbook
tb	469.52	K	Joback Method
tc	660.02	K	Joback Method
tf	253.97	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.56	J/mol×K	469.52	Joback Method
cpg	296.31	J/mol×K	628.27	Joback Method
cpg	287.63	J/mol×K	596.52	Joback Method
cpg	278.52	J/mol×K	564.77	Joback Method
cpg	268.98	J/mol×K	533.02	Joback Method
cpg	258.99	J/mol×K	501.27	Joback Method
cpg	304.57	J/mol×K	660.02	Joback Method
dvisc	0.0002704	Pa×s	469.52	Joback Method

dvisc	0.0003512	Pa×s	433.60	Joback Method
dvisc	0.0004783	Pa×s	397.67	Joback Method
dvisc	0.0006924	Pa×s	361.75	Joback Method
dvisc	0.0010878	Pa×s	325.82	Joback Method
dvisc	0.0019112	Pa×s	289.89	Joback Method
dvisc	0.0039384	Pa×s	253.97	Joback Method

Sources

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=R26546&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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