3-Buten-1-ol, chloroacetate

Inchi: InChI=1S/C6H9ClO2/c1-2-3-4-9-6(8)5-7/h2H,1,3-5H2
InchiKey: IYUCKRIJZHJOAQ-UHFFFAOYSA-N
Formula: C6H9ClO2
SMILES: C=CCCOC(=O)CCl
Mol. weight [g/mol]: 148.59

Physical Properties

Property code	Value	Unit	Source
gf	-158.37	kJ/mol	Joback Method
hf	-302.28	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	41.82	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.345		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	969.00		NIST Webbook
ripol	1504.00		NIST Webbook
tb	447.08	K	Joback Method
tc	635.32	K	Joback Method
tf	257.70	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.87	J/mol×K	447.08	Joback Method
cpg	217.78	J/mol×K	478.45	Joback Method
cpg	226.33	J/mol×K	509.83	Joback Method
cpg	234.52	J/mol×K	541.20	Joback Method
cpg	242.35	J/mol×K	572.57	Joback Method
cpg	249.84	J/mol×K	603.95	Joback Method
cpg	256.98	J/mol×K	635.32	Joback Method
dvisc	0.0027648	Pa×s	257.70	Joback Method

dvisc	0.0015611	Pa×s	289.26	Joback Method
dvisc	0.0009864	Pa×s	320.83	Joback Method
dvisc	0.0006767	Pa×s	352.39	Joback Method
dvisc	0.0004939	Pa×s	383.95	Joback Method
dvisc	0.0003781	Pa×s	415.52	Joback Method
dvisc	0.0003006	Pa×s	447.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26411&Units=SI

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