1-Chloro-3-methoxypropan-2-yl acetate

Other names: 2-Propanol, 1-chloro-3-methoxy-, acetate
Inchi: InChI=1S/C6H11ClO3/c1-5(8)10-6(3-7)4-9-2/h6H,3-4H2,1-2H3
InchiKey: KYQXJEOUFXTRCZ-UHFFFAOYSA-N
Formula: C6H11ClO3
SMILES: COCC(CCl)OC(C)=O
Mol. weight [g/mol]: 166.60

Physical Properties

Property code	Value	Unit	Source
gf	-353.65	kJ/mol	Joback Method
hf	-565.21	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	44.51	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.803		Crippen Method
mcvol	120.950	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	1075.00		NIST Webbook
rinpol	1075.00		NIST Webbook
tb	472.38	K	Joback Method
tc	660.04	K	Joback Method
tf	266.69	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.79	J/mol×K	472.38	Joback Method
cpg	292.50	J/mol×K	628.76	Joback Method
cpg	284.03	J/mol×K	597.49	Joback Method
cpg	275.21	J/mol×K	566.21	Joback Method
cpg	266.06	J/mol×K	534.93	Joback Method
cpg	256.58	J/mol×K	503.66	Joback Method
cpg	300.62	J/mol×K	660.04	Joback Method

dvisc	0.0002394	Pa×s	472.38	Joback Method
dvisc	0.0003108	Pa×s	438.10	Joback Method
dvisc	0.0004217	Pa×s	403.82	Joback Method
dvisc	0.0006055	Pa×s	369.53	Joback Method
dvisc	0.0009362	Pa×s	335.25	Joback Method
dvisc	0.0015986	Pa×s	300.97	Joback Method
dvisc	0.0031323	Pa×s	266.69	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=U373444&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume