2-Propenoic acid, 3-hydroxy-2-methyl-, ethyl ester

Inchi: InChI=1S/C6H10O3/c1-3-9-6(8)5(2)4-7/h4,7H,3H2,1-2H3/b5-4+
InchiKey: UPWSFLJBKRQKBD-SNAWJCMRSA-N
Formula: C6H10O3
SMILES: CCOC(=O)C(C)=CO
Mol. weight [g/mol]: 130.14
CAS: 54843-13-9

Physical Properties

Property code	Value	Unit	Source
gf	-299.43	kJ/mol	Joback Method
hf	-456.77	kJ/mol	Joback Method
hfus	17.06	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	1.011		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
tb	509.19	K	Joback Method
tc	690.58	K	Joback Method
tf	271.32	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.19	J/mol×K	509.19	Joback Method
cpg	235.61	J/mol×K	539.42	Joback Method
cpg	243.67	J/mol×K	569.65	Joback Method
cpg	251.38	J/mol×K	599.88	Joback Method
cpg	258.74	J/mol×K	630.12	Joback Method
cpg	265.76	J/mol×K	660.35	Joback Method
cpg	272.45	J/mol×K	690.58	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=C54843139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume