2-Butenoic acid, 3-hydroxy-, methyl ester, (E)-

Inchi: InChI=1S/C5H8O3/c1-4(6)3-5(7)8-2/h3,6H,1-2H3/b4-3-
InchiKey: DHVOJYDALVUWPZ-ARJAWSKDSA-N
Formula: C5H8O3
SMILES: COC(=O)C=C(C)O
Mol. weight [g/mol]: 116.12
CAS: 4525-24-0

Physical Properties

Property code	Value	Unit	Source
gf	-307.85	kJ/mol	Joback Method
hf	-436.13	kJ/mol	Joback Method
hfus	14.47	kJ/mol	Joback Method
hvap	52.60	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.621		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	486.31	K	Joback Method
tc	669.55	K	Joback Method
tf	260.05	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.77	J/mol×K	486.31	Joback Method
cpg	194.05	J/mol×K	516.85	Joback Method
cpg	201.03	J/mol×K	547.39	Joback Method
cpg	207.70	J/mol×K	577.93	Joback Method
cpg	214.07	J/mol×K	608.47	Joback Method
cpg	220.15	J/mol×K	639.01	Joback Method
cpg	225.95	J/mol×K	669.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4525240&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
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