methyl 4-hydroxy-3-methyl-2-pentenoate

Inchi: InChI=1S/C7H12O3/c1-5(6(2)8)4-7(9)10-3/h4,6,8H,1-3H3/b5-4+
InchiKey: HIPRDLZWAASLOU-SNAWJCMRSA-N
Formula: C7H12O3
SMILES: COC(=O)C=C(C)C(C)O
Mol. weight [g/mol]: 144.17
CAS: 102539-97-9

Physical Properties

Property code	Value	Unit	Source
gf	-293.45	kJ/mol	Joback Method
hf	-482.69	kJ/mol	Joback Method
hfus	16.13	kJ/mol	Joback Method
hvap	56.66	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	0.486		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
tb	531.63	K	Joback Method
tc	714.80	K	Joback Method
tf	267.59	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.97	J/mol×K	531.63	Joback Method
cpg	279.67	J/mol×K	562.16	Joback Method
cpg	288.94	J/mol×K	592.69	Joback Method
cpg	297.78	J/mol×K	623.22	Joback Method
cpg	306.21	J/mol×K	653.74	Joback Method
cpg	314.23	J/mol×K	684.27	Joback Method
cpg	321.86	J/mol×K	714.80	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=C102539979&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume