3-Pentenoic acid, 2-hydroxymethylene-4-methyl-, methyl ester

Inchi: InChI=1S/C8H12O3/c1-6(2)4-7(5-9)8(10)11-3/h4-5,9H,1-3H3/b7-5+

InchiKey: FTXSRGLQMZZFQL-FNORWQNLSA-N

Formula: C8H12O3

SMILES: COC(=O)C(C=C(C)C)=CO

Mol. weight [g/mol]: 156.18

CAS: 90199-77-2

Physical Properties

Property code	Value	Unit	Source
gf	-210.92	kJ/mol	Joback Method
hf	-390.62	kJ/mol	Joback Method
hfus	21.14	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.567		Crippen Method
mcvol	128.290	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	558.99	K	Joback Method
tc	747.20	K	Joback Method
tf	274.82	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.37	J/mol×K	558.99	Joback Method
cpg	304.32	J/mol×K	590.36	Joback Method
cpg	313.76	J/mol×K	621.73	Joback Method
cpg	322.72	J/mol×K	653.10	Joback Method
cpg	331.22	J/mol×K	684.47	Joback Method
cpg	339.28	J/mol×K	715.83	Joback Method
cpg	346.93	J/mol×K	747.20	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=C90199772&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