Pentanoic acid, 2,4-dioxo-, methyl ester

Other names: methyl acetopyruvate
Inchi: InChI=1S/C6H8O4/c1-4(7)3-5(8)6(9)10-2/h3H2,1-2H3
InchiKey: OMHOEQINEXASKE-UHFFFAOYSA-N
Formula: C6H8O4
SMILES: COC(=O)C(=O)CC(C)=O
Mol. weight [g/mol]: 144.13
CAS: 20577-61-1

Physical Properties

Property code	Value	Unit	Source
gf	-492.12	kJ/mol	Joback Method
hf	-637.13	kJ/mol	Joback Method
hfus	17.28	kJ/mol	Joback Method
hvap	51.60	kJ/mol	Joback Method
log10ws	0.24		Crippen Method
logp	-0.292		Crippen Method
mcvol	105.980	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	520.71	K	Joback Method
tc	719.19	K	Joback Method
tf	329.40	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.36	J/mol×K	520.71	Joback Method
cpg	236.04	J/mol×K	553.79	Joback Method
cpg	244.33	J/mol×K	586.87	Joback Method
cpg	252.25	J/mol×K	619.95	Joback Method
cpg	259.79	J/mol×K	653.03	Joback Method
cpg	266.93	J/mol×K	686.11	Joback Method
cpg	273.68	J/mol×K	719.19	Joback Method
dvisc	0.0023960	Pa×s	329.40	Joback Method

dvisc	0.0015048	Pa×s	361.29	Joback Method
dvisc	0.0010192	Pa×s	393.17	Joback Method
dvisc	0.0007318	Pa×s	425.06	Joback Method
dvisc	0.0005503	Pa×s	456.94	Joback Method
dvisc	0.0004295	Pa×s	488.83	Joback Method
dvisc	0.0003456	Pa×s	520.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20577611&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume