5-Methylhexane-2,4-dione, keto form

Other names: 5-Methyl-2,4-hexanedione (enol)
5-Methyl-2,4-hexanedione
Inchi: InChI=1S/C7H12O2/c1-5(2)7(9)4-6(3)8/h5H,4H2,1-3H3
InchiKey: KHZGUWAFFHXZLC-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: CC(=O)CC(=O)C(C)C
Mol. weight [g/mol]: 128.17
CAS: 7307-03-1

Physical Properties

Property code	Value	Unit	Source
gf	-252.22	kJ/mol	Joback Method
hf	-452.70	kJ/mol	NIST Webbook
hfus	13.56	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.191		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	940.17		NIST Webbook
rinpol	940.17		NIST Webbook
rinpol	950.54		NIST Webbook
rinpol	945.33		NIST Webbook
rinpol	944.07		NIST Webbook
tb	466.86	K	Joback Method
tc	658.82	K	Joback Method
tf	253.51	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.52	J/mol×K	466.86	Joback Method
cpg	244.55	J/mol×K	498.85	Joback Method

cpg	255.07	J/mol×K	530.85	Joback Method
cpg	265.11	J/mol×K	562.84	Joback Method
cpg	274.67	J/mol×K	594.83	Joback Method
cpg	283.77	J/mol×K	626.83	Joback Method
cpg	292.41	J/mol×K	658.82	Joback Method
dvisc	0.0049833	Pa×s	253.51	Joback Method
dvisc	0.0024070	Pa×s	289.07	Joback Method
dvisc	0.0013635	Pa×s	324.63	Joback Method
dvisc	0.0008641	Pa×s	360.19	Joback Method
dvisc	0.0005944	Pa×s	395.74	Joback Method
dvisc	0.0004349	Pa×s	431.30	Joback Method
dvisc	0.0003337	Pa×s	466.86	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=C7307031&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume