2-Hydroxy-2,4-dimethyl-3-pentanone

Other names: 3-Pentanone, 2-hydroxy-2,4-dimethyl-
Inchi: InChI=1S/C7H14O2/c1-5(2)6(8)7(3,4)9/h5,9H,1-4H3
InchiKey: XWJXXDDXZUVWBY-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CC(C)C(=O)C(C)(C)O
Mol. weight [g/mol]: 130.18
CAS: 3212-67-7

Physical Properties

Property code	Value	Unit	Source
gf	-257.28	kJ/mol	Joback Method
hf	-466.65	kJ/mol	Joback Method
hfus	8.64	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.982		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
ripol	1376.00		NIST Webbook
ripol	1376.00		NIST Webbook
tb	501.94	K	Joback Method
tc	685.54	K	Joback Method
tf	266.82	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.14	J/mol×K	501.94	Joback Method
cpg	280.15	J/mol×K	532.54	Joback Method
cpg	290.58	J/mol×K	563.14	Joback Method
cpg	300.44	J/mol×K	593.74	Joback Method
cpg	309.77	J/mol×K	624.34	Joback Method
cpg	318.59	J/mol×K	654.94	Joback Method

cpg	326.92	J/mol×K	685.54	Joback Method
dvisc	0.0460707	Pa×s	266.82	Joback Method
dvisc	0.0098531	Pa×s	306.01	Joback Method
dvisc	0.0029909	Pa×s	345.19	Joback Method
dvisc	0.0011577	Pa×s	384.38	Joback Method
dvisc	0.0005342	Pa×s	423.57	Joback Method
dvisc	0.0002810	Pa×s	462.75	Joback Method
dvisc	0.0001634	Pa×s	501.94	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=C3212677&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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