2-Pentanone, 3,3,4,4-tetramethyl-

Inchi: InChI=1S/C9H18O/c1-7(10)9(5,6)8(2,3)4/h1-6H3
InchiKey: VVCKMVBQLNBXOE-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CC(=O)C(C)(C)C(C)(C)C
Mol. weight [g/mol]: 142.24
CAS: 865-66-7

Physical Properties

Property code	Value	Unit	Source
gf	-98.34	kJ/mol	Joback Method
hf	-347.70 ± 1.80	kJ/mol	NIST Webbook
hfus	5.84	kJ/mol	Joback Method
hvap	39.78	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.648		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
tb	441.00 ± 5.00	K	NIST Webbook
tb	446.00 ± 6.00	K	NIST Webbook
tb	441.00 ± 4.00	K	NIST Webbook
tb	441.00 ± 8.00	K	NIST Webbook
tc	649.78	K	Joback Method
tf	334.00 ± 6.00	K	NIST Webbook
tf	335.00 ± 3.00	K	NIST Webbook
tf	331.90 ± 2.00	K	NIST Webbook
tf	337.00 ± 2.00	K	NIST Webbook
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.55	J/mol×K	452.73	Joback Method
cpg	318.74	J/mol×K	485.57	Joback Method
cpg	333.95	J/mol×K	518.41	Joback Method

cpg	348.22	J/mol×K	551.25	Joback Method
cpg	361.62	J/mol×K	584.10	Joback Method
cpg	374.18	J/mol×K	616.94	Joback Method
cpg	385.96	J/mol×K	649.78	Joback Method
dvisc	0.0097546	Pa×s	245.96	Joback Method
dvisc	0.0038032	Pa×s	280.42	Joback Method
dvisc	0.0018223	Pa×s	314.88	Joback Method
dvisc	0.0010096	Pa×s	349.35	Joback Method
dvisc	0.0006219	Pa×s	383.81	Joback Method
dvisc	0.0004149	Pa×s	418.27	Joback Method
dvisc	0.0002944	Pa×s	452.73	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=C865667&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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