2-Heptanone, 4,6-dimethyl-

Other names: 4,6-dimethyl-2-heptanone
4,6-dimethylheptan-2-one
Inchi: InChI=1S/C9H18O/c1-7(2)5-8(3)6-9(4)10/h7-8H,5-6H2,1-4H3
InchiKey: YXFDTUKUWNQPFV-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CC(=O)CC(C)CC(C)C
Mol. weight [g/mol]: 142.24
CAS: 19549-80-5

Physical Properties

Property code	Value	Unit	Source
gf	-108.90	kJ/mol	Joback Method
hf	-352.23	kJ/mol	Joback Method
hfus	13.62	kJ/mol	Joback Method
hvap	41.60	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.648		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1045.00		NIST Webbook
rinpol	979.90		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	979.90		NIST Webbook
ripol	1262.40		NIST Webbook
ripol	1262.40		NIST Webbook
tb	464.00 ± 4.00	K	NIST Webbook
tc	640.10	K	Joback Method
tf	211.12	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.92	J/mol×K	458.31	Joback Method

cpg	312.19	J/mol×K	488.61	Joback Method
cpg	325.86	J/mol×K	518.91	Joback Method
cpg	338.94	J/mol×K	549.20	Joback Method
cpg	351.45	J/mol×K	579.50	Joback Method
cpg	363.40	J/mol×K	609.80	Joback Method
cpg	374.81	J/mol×K	640.10	Joback Method
dvisc	0.0112700	Pa×s	211.12	Joback Method
dvisc	0.0035885	Pa×s	252.32	Joback Method
dvisc	0.0015755	Pa×s	293.52	Joback Method
dvisc	0.0008471	Pa×s	334.72	Joback Method
dvisc	0.0005218	Pa×s	375.91	Joback Method
dvisc	0.0003537	Pa×s	417.11	Joback Method
dvisc	0.0002572	Pa×s	458.31	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Quaternary phase equilibrium of water-carboxylic acid mixture (formic-propionic acid or acetic-propionic acid)-solvent liquid systems at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2011.09.014
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=C19549805&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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