3-Hexanone, 2,4-dimethyl-

Other names: 2,4-Dimethyl-3-hexanone
2,4-Dimethyl hexanone-3
Inchi: InChI=1S/C8H16O/c1-5-7(4)8(9)6(2)3/h6-7H,5H2,1-4H3
InchiKey: PZAPVPGZDHJUTO-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCC(C)C(=O)C(C)C
Mol. weight [g/mol]: 128.21
CAS: 18641-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-117.32	kJ/mol	Joback Method
hf	-331.59	kJ/mol	Joback Method
hfus	11.03	kJ/mol	Joback Method
hvap	39.37	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	2.258		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
ripol	1178.00		NIST Webbook
ripol	1178.00		NIST Webbook
tb	421.00 ± 2.00	K	NIST Webbook
tb	420.00 ± 2.00	K	NIST Webbook
tb	418.00 ± 3.00	K	NIST Webbook
tc	618.82	K	Joback Method
tf	199.85	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.99	J/mol×K	618.82	Joback Method
cpg	255.61	J/mol×K	435.43	Joback Method
cpg	268.85	J/mol×K	466.00	Joback Method

cpg	281.53	J/mol×K	496.56	Joback Method
cpg	293.67	J/mol×K	527.13	Joback Method
cpg	305.29	J/mol×K	557.69	Joback Method
cpg	316.39	J/mol×K	588.26	Joback Method
dvisc	0.0002700	Pa×s	435.43	Joback Method
dvisc	0.0114893	Pa×s	199.85	Joback Method
dvisc	0.0036803	Pa×s	239.11	Joback Method
dvisc	0.0016253	Pa×s	278.38	Joback Method
dvisc	0.0008785	Pa×s	317.64	Joback Method
dvisc	0.0005437	Pa×s	356.90	Joback Method
dvisc	0.0003700	Pa×s	396.17	Joback Method
hvapt	42.50	kJ/mol	384.00	NIST Webbook

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=C18641708&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
hvapt: Enthalpy of vaporization at a given temperature
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