3-Hexanone, 2,5-dimethyl-

Other names: 2,5-Dimethyl-3-hexanone
Isobutyl isopropyl ketone
Inchi: InChI=1S/C8H16O/c1-6(2)5-8(9)7(3)4/h6-7H,5H2,1-4H3
InchiKey: TUIWMHDSXJWXOH-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CC(C)CC(=O)C(C)C
Mol. weight [g/mol]: 128.21
CAS: 1888-57-9

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	1145.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1145.00		NIST Webbook
tb	416.00 ± 4.00	K	NIST Webbook
tb	466.00 ± 30.00	K	NIST Webbook
tb	420.70	K	NIST Webbook
tb	421.00 ± 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	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
cpg	326.99	J/mol×K	618.82	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
dvisc	0.0002700	Pa×s	435.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50079e+01
Coeff. B	-3.76736e+03
Coeff. C	-5.80910e+01
Temperature range (K), min.	314.02
Temperature range (K), max.	446.62

Sources

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=C1888579&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume