3-Hexanone, 2,2-dimethyl-

Other names: 2,2-DIMETHYLHEXAN-3-ONE
2,2-Dimethyl-3-hexanone
tert-Butyl Propyl ketone
Inchi: InChI=1S/C8H16O/c1-5-6-7(9)8(2,3)4/h5-6H2,1-4H3
InchiKey: PYCHXHVFOZBVEY-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCCC(=O)C(C)(C)C
Mol. weight [g/mol]: 128.21
CAS: 5405-79-8

Physical Properties

Property code	Value	Unit	Source
gf	-109.60	kJ/mol	Joback Method
hf	-329.78	kJ/mol	Joback Method
hfus	10.66	kJ/mol	Joback Method
hvap	38.85	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	420.00 ± 3.00	K	NIST Webbook
tb	417.00 ± 3.00	K	NIST Webbook
tb	420.00 ± 3.00	K	NIST Webbook
tb	419.00 ± 2.00	K	NIST Webbook
tc	619.80	K	Joback Method
tf	232.27	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.73	J/mol×K	433.08	Joback Method
cpg	320.09	J/mol×K	588.68	Joback Method
cpg	308.91	J/mol×K	557.56	Joback Method

cpg	297.11	J/mol×K	526.44	Joback Method
cpg	284.66	J/mol×K	495.32	Joback Method
cpg	271.54	J/mol×K	464.20	Joback Method
cpg	330.68	J/mol×K	619.80	Joback Method
dvisc	0.0003081	Pa×s	433.08	Joback Method
dvisc	0.0004158	Pa×s	399.61	Joback Method
dvisc	0.0005927	Pa×s	366.14	Joback Method
dvisc	0.0009076	Pa×s	332.67	Joback Method
dvisc	0.0015286	Pa×s	299.21	Joback Method
dvisc	0.0029357	Pa×s	265.74	Joback Method
dvisc	0.0068051	Pa×s	232.27	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50249e+01
Coeff. B	-3.76017e+03
Coeff. C	-5.76740e+01
Temperature range (K), min.	312.82
Temperature range (K), max.	444.78

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=C5405798&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

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