

3-Hexanone, 4-methyl-

Other names:	4-Methyl-3-hexanone 4-Methylhexan-3-one Ethyl sec-butyl ketone sec-butyl ethyl ketone
Inchi:	InChI=1S/C7H14O/c1-4-6(3)7(8)5-2/h6H,4-5H2,1-3H3
InchiKey:	ULPMRIXXHGUZFA-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCC(=O)C(C)CC
Mol. weight [g/mol]:	114.19
CAS:	17042-16-9

Physical Properties

Property code	Value	Unit	Source
gf	-123.30	kJ/mol	Joback Method
hf	-305.67	kJ/mol	Joback Method
hfus	11.96	kJ/mol	Joback Method
hvap	37.53	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	2.012		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	804.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	842.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1079.00		NIST Webbook
tb	412.99	K	Joback Method
tc	593.63	K	Joback Method
tf	203.58	K	Joback Method
vc	0.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.47	J/molxK	412.99	Joback Method
cpg	269.42	J/molxK	563.52	Joback Method
cpg	259.52	J/molxK	533.42	Joback Method
cpg	249.19	J/molxK	503.31	Joback Method
cpg	238.41	J/molxK	473.20	Joback Method
cpg	227.17	J/molxK	443.10	Joback Method
cpg	278.88	J/molxK	593.63	Joback Method
dvisc	0.0002897	Paxs	412.99	Joback Method
dvisc	0.0003833	Paxs	378.09	Joback Method
dvisc	0.0005371	Paxs	343.19	Joback Method
dvisc	0.0008121	Paxs	308.28	Joback Method
dvisc	0.0013648	Paxs	273.38	Joback Method
dvisc	0.0026700	Paxs	238.48	Joback Method
dvisc	0.0065747	Paxs	203.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47279e+01
Coeff. B	-3.60901e+03
Coeff. C	-5.48940e+01
Temperature range (K), min.	304.82
Temperature range (K), max.	438.16

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C17042169&Units=SI>

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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>

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
mccvol: McGowan's characteristic volume
pc: Critical Pressure
pvap: Vapor 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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