

Cyclohexanone, 2-methyl-

Other names:	2-Methyl-1-cyclohexanone 2-Methyl-cyclohexanon 2-Methylcyclohexanone 2-Metilcicloesanone o-Methylcyclohexanone «alpha»-Methylcyclohexanone Â«alphaÂ»-Methylcyclohexanone
Inchi:	InChI=1S/C7H12O/c1-6-4-2-3-5-7(6)8/h6H,2-5H2,1H3
InchiKey:	LFSAPCRASZRSKS-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CC1CCCCC1=O
Mol. weight [g/mol]:	112.17
CAS:	583-60-8

Physical Properties

Property code	Value	Unit	Source
ea	0.00 ± 0.00	eV	NIST Webbook
gf	-90.08	kJ/mol	Joback Method
hf	-271.19	kJ/mol	Joback Method
hfus	5.23	kJ/mol	Joback Method
hvap	44.00	kJ/mol	NIST Webbook
ie	9.50 ± 0.20	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
log10ws	-0.94		Aqueous Solubility Prediction Method
logp	1.766		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	932.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	953.10		NIST Webbook
rinpol	930.00		NIST Webbook

rinpol	935.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	949.00		NIST Webbook
tb	373.40 ± 0.80	K	NIST Webbook
tb	439.00 ± 6.00	K	NIST Webbook
tb	391.65 ± 0.25	K	NIST Webbook
tb	435.70	K	NIST Webbook
tb	438.20 ± 0.50	K	NIST Webbook
tc	670.65	K	Joback Method
tf	256.00 ± 6.00	K	NIST Webbook
tf	264.00 ± 2.00	K	NIST Webbook
tf	259.25 ± 0.40	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.79	J/mol×K	484.22	Joback Method
cpg	288.21	J/mol×K	670.65	Joback Method
cpg	275.92	J/mol×K	633.36	Joback Method
cpg	262.92	J/mol×K	596.07	Joback Method
cpg	249.23	J/mol×K	558.79	Joback Method
cpg	234.85	J/mol×K	521.50	Joback Method
cpg	204.07	J/mol×K	446.93	Joback Method
cpl	204.60	J/mol×K	290.00	NIST Webbook
hvapt	45.00	kJ/mol	384.00	NIST Webbook
pvap	9.54	kPa	363.09	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	10.98	kPa	366.66	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	12.30	kPa	369.65	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	13.79	kPa	372.70	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one

pvap	15.79	kPa	376.36	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	19.12	kPa	381.72	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	21.37	kPa	384.91	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	8.68	kPa	360.73	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	29.53	kPa	394.59	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	33.29	kPa	398.32	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	35.05	kPa	399.98	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	45.03	kPa	408.17	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	49.98	kPa	411.64	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	53.52	kPa	414.00	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	60.46	kPa	418.28	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	99.71	kPa	436.94	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one

pvap	7.94	kPa	358.53	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	7.13	kPa	355.93	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	6.40	kPa	353.34	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	5.76	kPa	350.96	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	5.27	kPa	348.85	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	3.91	kPa	342.20	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	3.33	kPa	338.76	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	24.90	kPa	389.42	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42147e+01
Coeff. B	-3.60437e+03
Coeff. C	-6.25530e+01
Temperature range (K), min.	285.48
Temperature range (K), max.	467.39

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one:	https://www.doi.org/10.1021/je0504358
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C583608&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
ea:	Electron affinity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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