

2-Cyclohexen-1-one

Other names:	1-Cyclohexen-3-one
	2-Cyclohexene-1-one
	2-Cyclohexenone-1
	2-cyclohexenone
	Cyclohex-2-en-1-one
	Cyclohexen-2-one
	Cyclohexen-3-one
	cyclohex-2-enone
	cyclohexenone
Inchi:	InChI=1S/C6H8O/c7-6-4-2-1-3-5-6/h2,4H,1,3,5H2
InchiKey:	FWFSEYBSWVRWGL-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	O=C1C=CCCC1
Mol. weight [g/mol]:	96.13
CAS:	930-68-7

Physical Properties

Property code	Value	Unit	Source
gf	-60.83	kJ/mol	Joback Method
hf	-172.43	kJ/mol	Joback Method
hfus	2.79	kJ/mol	Joback Method
hvap	49.50 ± 0.40	kJ/mol	NIST Webbook
ie	9.37	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.23 ± 0.05	eV	NIST Webbook
log10ws	-1.36		Crippen Method
logp	1.296		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
pc	4530.00 ± 250.00	kPa	NIST Webbook
rhoc	315.30 ± 20.19	kg/m3	NIST Webbook
rinpol	136.20		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	914.00		NIST Webbook

ripol	1413.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1412.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1437.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1437.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1412.00		NIST Webbook
ripol	1437.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1462.00		NIST Webbook
ripol	1433.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1412.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1422.00		NIST Webbook
tb	440.50 ± 0.50	K	NIST Webbook
tb	443.20	K	NIST Webbook
tb	441.20	K	NIST Webbook
tc	685.00 ± 6.00	K	NIST Webbook
tf	237.98	K	Joback Method
vc	0.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.60	J/mol×K	466.18	Joback Method
cpg	215.77	J/mol×K	657.68	Joback Method
cpg	206.12	J/mol×K	619.38	Joback Method
cpg	195.87	J/mol×K	581.08	Joback Method
cpg	185.03	J/mol×K	542.78	Joback Method
cpg	173.60	J/mol×K	504.48	Joback Method
cpg	149.01	J/mol×K	427.88	Joback Method
hvapt	45.00	kJ/mol	398.00	NIST Webbook

pvap	35.56	kPa	407.95	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	17.53	kPa	386.63	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	18.68	kPa	388.40	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	20.95	kPa	391.77	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	25.20	kPa	397.16	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	32.03	kPa	404.53	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	14.06	kPa	380.50	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	39.01	kPa	410.86	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	57.64	kPa	424.23	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	100.40	kPa	445.00	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	99.00	kPa	444.48	Vapor-Liquid Equilibria of Cyclohexanone + 2-Cyclohexen-1-one and Cyclohexanol + 2-Cyclohexen-1-one, Validated in a Packed Column Distillation.

pvap	99.00	kPa	444.51	Vapor-Liquid Equilibria of Cyclohexanone + 2-Cyclohexen-1-one and Cyclohexanol + 2-Cyclohexen-1-one, Validated in a Packed Column Distillation.
pvap	13.31	kPa	379.00	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	11.46	kPa	374.97	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	9.58	kPa	370.32	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	8.10	kPa	366.16	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	6.71	kPa	361.48	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	5.66	kPa	357.56	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	4.79	kPa	353.66	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one
pvap	4.15	kPa	350.40	Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one

Sources

Crippen Method:

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

Vapor Pressures of Hexanal, 2-Methylcyclohexanone, and 2-Cyclohexen-1-one:

<https://www.doi.org/10.1021/je0504358>

Vapor-Liquid Equilibria of
Cyclohexanone + 2-Cyclohexen-1-one
and Cyclohexanol +
2-Cyclohexen-1-one, Validated in a
Packed Column Distillation.:
NIST Webbook:
Crippen Method:

<https://www.doi.org/10.1021/je501135p>
https://en.wikipedia.org/wiki/Joback_method
<http://link.springer.com/article/10.1007/BF02311772>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C930687&Units=SI>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

cpg:	Ideal gas heat capacity
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
rhoc:	Critical density
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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