Cyclohexanol, 1-methyl-

Other names:	1-METHYL-1-CYCLOHEXANOL
	1-Methylcyclohexanol
Inchi:	InChI=1S/C7H14O/c1-7(8)5-3-2-4-6-7/h8H,2-6H2,1H3
InchiKey:	VTBOTOBFGSVRMA-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CC1(O)CCCCC1
Mol. weight [g/mol]:	114.19
CAS:	590-67-0

Physical Properties

Property code	Value	Unit	Source
gf	-109.80	kJ/mol	Joback Method
hf	-270.48	kJ/mol	Joback Method
hfs	-391.90 ± 0.80	kJ/mol	NIST Webbook
hfus	3.51	kJ/mol	Joback Method
hvap	47.13	kJ/mol	Joback Method
ie	9.80 ± 0.20	eV	NIST Webbook
log10ws	-2.02		Crippen Method
logp	1.701		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	4173.09	kPa	Joback Method
rinpol	868.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
tb	427.15 ± 2.00	K	NIST Webbook
tb	428.20	K	NIST Webbook
tb	438.65 ± 1.50	K	NIST Webbook
tc	672.52	K	Joback Method
tf	297.90 ± 1.50	K	NIST Webbook
tf	299.10 ± 2.00	K	NIST Webbook
tt	299.40 ± 0.15	K	NIST Webbook
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.77	J/mol×K	639.02	Joback Method
cpg	231.11	J/mol×K	471.53	Joback Method
cpg	245.11	J/mol×K	505.03	Joback Method
cpg	258.19	J/mol×K	538.53	Joback Method
cpg	270.43	J/mol×K	572.03	Joback Method
cpg	281.93	J/mol×K	605.52	Joback Method
cpg	303.04	J/mol×K	672.52	Joback Method
cpl	279.05	J/mol×K	298.15	NIST Webbook
hfust	10.87	kJ/mol	299.20	NIST Webbook
hfust	14.32	kJ/mol	299.40	NIST Webbook
hfust	10.87	kJ/mol	299.20	NIST Webbook
hsubt	75.90 ± 0.40	kJ/mol	291.00	NIST Webbook
hvapt	49.10	kJ/mol	385.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.20	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61238e+01
Coeff. B	-4.23413e+03
Coeff. C	-6.01900e+01
Temperature range (K), min.	299.15
Temperature range (K), max.	451.79

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.45806e+02
Coeff. B	-1.21502e+04
Coeff. C	-1.89544e+01
Coeff. D	1.07872e-05
Temperature range (K), min.	299.15
Temperature range (K), max.	603.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol901.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590670&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=901

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume