Cyclohexanol, 2-methyl-

Other names:	1-Methyl-2-cyclohexanol
	2-Methyl-1-cyclohexanol
	2-Methylcyclohexanol
	2-Methylcyclohexyl alcohol
	2-methylcyclohexanol, mixed isomers
	Cyclohexanol, o-methyl-
	NSC 75845
	o-Methylcyclohexanol
Inchi:	InChI=1S/C7H14O/c1-6-4-2-3-5-7(6)8/h6-8H,2-5H2,1H3
InchiKey:	NDVWOBYBJYUSMF-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CC1CCCCC1O
Mol. weight [g/mol]:	114.19
CAS:	583-59-5

Physical Properties

Property code	Value	Unit	Source
chl	-4380.20	kJ/mol	NIST Webbook
gf	-112.02	kJ/mol	Joback Method
hf	-306.06	kJ/mol	Joback Method
hfus	10.88	kJ/mol	Joback Method
hvap	63.30	kJ/mol	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.557		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	973.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	946.00		NIST Webbook
tb	441.65 ± 0.50	K	NIST Webbook
tb	437.70	K	NIST Webbook
tb	440.70 ± 1.00	K	NIST Webbook
tc	659.09	K	Joback Method
tf	232.61	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.10	J/mol×K	659.09	Joback Method
cpg	284.31	J/mol×K	594.94	Joback Method
cpg	271.99	J/mol×K	562.86	Joback Method
cpg	259.05	J/mol×K	530.78	Joback Method
cpg	245.46	J/mol×K	498.70	Joback Method
cpg	231.22	J/mol×K	466.62	Joback Method
cpg	296.01	J/mol×K	627.01	Joback Method
cpl	267.44	J/mol×K	298.15	NIST Webbook
cpl	199.60	J/mol×K	290.00	NIST Webbook
dvisc	0.0550246	Pa×s	232.61	Joback Method
dvisc	0.0112900	Pa×s	271.61	Joback Method
dvisc	0.0034480	Pa×s	310.61	Joback Method
dvisc	0.0013721	Pa×s	349.62	Joback Method
dvisc	0.0006569	Pa×s	388.62	Joback Method
dvisc	0.0003597	Pa×s	427.62	Joback Method
dvisc	0.0002179	Pa×s	466.62	Joback Method
hvapt	51.70	kJ/mol	400.00	NIST Webbook
rfi	1.46313		293.10	Vapor-Liquid Equilibria in the 2-Methylcyclohexanol + 2-Methylcyclohexyl Ethanoate System at 101.325 kPa
srf	0.03	N/m	323.15	Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols
srf	0.03	N/m	308.15	Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols
srf	0.03	N/m	303.15	Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols

srf	0.03	N/m	298.15	Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols
srf	0.03	N/m	293.15	Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols
srf	0.03	N/m	318.15	Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols
srf	0.03	N/m	313.15	Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.70042e+01
Coeff. B	-4.61743e+03
Coeff. C	-6.49020e+01
Temperature range (K), min.	341.12
Temperature range (K), max.	459.80

Sources

Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols:	https://www.doi.org/10.1021/je049919e
Vapor-Liquid Equilibria in the 2-Methylcyclohexanol + 2-Methylcyclohexyl Ethanoate System at 101.325 kPa:	https://www.doi.org/10.1021/je600559q
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=C583595&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume