

Cyclohexanol, 4-methyl-

Other names:	1-Methyl-4-cyclohexanol 4-Methylcyclohexanol 4-Methylcyclohexanol cis+trans 4-Methylcyclohexanol,c&t 4-methylcyclohexanol (cis+trans) 4-methylcyclohexanol, mixed isomers cyclohexanol, 4-methyl- (cis+trans) p-Methylcyclohexanol
Inchi:	InChI=1S/C7H14O/c1-6-2-4-7(8)5-3-6/h6-8H,2-5H2,1H3
InchiKey:	MQWCXKKGKQLNYQG-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CC1CCC(O)CC1
Mol. weight [g/mol]:	114.19
CAS:	589-91-3

Physical Properties

Property code	Value	Unit	Source
gf	-112.02	kJ/mol	Joback Method
hf	-306.06	kJ/mol	Joback Method
hfus	10.88	kJ/mol	Joback Method
hvap	65.90	kJ/mol	NIST Webbook
log10ws	-0.88		Aqueous Solubility Prediction Method
logp	1.557		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	941.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	926.00		NIST Webbook
tb	445.20	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/molxK	659.09	Joback Method
cpg	296.01	J/molxK	627.01	Joback Method
cpg	284.31	J/molxK	594.94	Joback Method
cpg	271.99	J/molxK	562.86	Joback Method
cpg	259.05	J/molxK	530.78	Joback Method
cpg	245.46	J/molxK	498.70	Joback Method
cpg	231.22	J/molxK	466.62	Joback Method
cpl	202.10	J/molxK	290.00	NIST Webbook
dvisc	0.0003597	Paxs	427.62	Joback Method
dvisc	0.0550246	Paxs	232.61	Joback Method
dvisc	0.0112900	Paxs	271.61	Joback Method
dvisc	0.0002179	Paxs	466.62	Joback Method
dvisc	0.0034480	Paxs	310.61	Joback Method
dvisc	0.0013721	Paxs	349.62	Joback Method
dvisc	0.0006569	Paxs	388.62	Joback Method
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	323.15	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

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	308.15	Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols

Sources

Surface Properties of Pure Liquids and Binary Liquid Mixtures of Ethylene Glycol + Methylcyclohexanols:	https://www.doi.org/10.1021/je049919e
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C589913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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
hvac:	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
rinpol:	Non-polar retention indices

srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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