

Cyclohexanol, 2-methyl-, trans-

Other names:	trans-2-Methylcyclohexanol
Inchi:	InChI=1S/C7H14O/c1-6-4-2-3-5-7(6)8/h6-8H,2-5H2,1H3/t6-,7-/m0/s1
InchiKey:	NDVWOBYBJYUSMF-BQBZGAKWSA-N
Formula:	C7H14O
SMILES:	CC1CCCCC1O
Mol. weight [g/mol]:	114.19
CAS:	7443-52-9

Physical Properties

Property code	Value	Unit	Source
chl	-4334.20 ± 3.30	kJ/mol	NIST Webbook
chl	-4322.20 ± 3.30	kJ/mol	NIST Webbook
gf	-112.02	kJ/mol	Joback Method
hf	-306.06	kJ/mol	Joback Method
hfl	-421.25	kJ/mol	NIST Webbook
hfus	10.88	kJ/mol	Joback Method
hvap	47.97	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.557		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	946.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1438.00		NIST Webbook
tb	440.60	K	NIST Webbook
tc	659.09	K	Joback Method
tf	232.61	K	Joback Method
vc	0.379	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.22	J/mol×K	466.62	Joback Method
cpg	296.01	J/mol×K	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	307.10	J/molxK	659.09	Joback Method
dvisc	0.0002179	Paxs	466.62	Joback Method
dvisc	0.0003597	Paxs	427.62	Joback Method
dvisc	0.0006569	Paxs	388.62	Joback Method
dvisc	0.0013721	Paxs	349.62	Joback Method
dvisc	0.0034480	Paxs	310.61	Joback Method
dvisc	0.0112900	Paxs	271.61	Joback Method
dvisc	0.0550246	Paxs	232.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60691e+01
Coeff. B	-4.31795e+03
Coeff. C	-6.35120e+01
Temperature range (K), min.	337.12
Temperature range (K), max.	464.90

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.61143e+01
Coeff. B	-8.61631e+03
Coeff. C	-8.68733e+00
Coeff. D	5.02864e-06
Temperature range (K), min.	269.15
Temperature range (K), max.	616.00

Sources

KDB:

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=903>

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7443529&Units=SI
The Yaws Handbook of Vapor Pressure: KDB Vapor Pressure Data:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=903
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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