

cis-3-Methylcyclohexanol

Other names:	3-Methyl cyclohexanol, cis 3-Methylcyclohexanol, (Z)- Cyclohexanol, 3-methyl-, cis-
Inchi:	InChI=1S/C7H14O/c1-6-3-2-4-7(8)5-6/h6-8H,2-5H2,1H3/t6-,7+/m0/s1
InchiKey:	HTSABYAWKQAHBT-NKWVEPMBSA-N
Formula:	C7H14O
SMILES:	CC1CCCC(O)C1
Mol. weight [g/mol]:	114.19
CAS:	5454-79-5

Physical Properties

Property code	Value	Unit	Source
chl	-4355.50 ± 3.30	kJ/mol	NIST Webbook
chl	-4334.70 ± 3.30	kJ/mol	NIST Webbook
gf	-112.02	kJ/mol	Joback Method
hf	-306.06	kJ/mol	Joback Method
hfl	-399.90	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
nfpaf	%!d(float64=2)		KDB
pc	3782.33	kPa	Joback Method
rinpola	964.00		NIST Webbook
ripola	1482.00		NIST Webbook
tb	466.62	K	Joback Method
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
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cpg	231.22	J/molxK	466.62	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	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	1.72389e+01
Coeff. B	-4.69110e+03
Coeff. C	-6.51800e+01
Temperature range (K), min.	341.92
Temperature range (K), max.	458.48

Sources

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<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.thermo.com/research/kdb/hcprop/showprop.php?cmpid=904>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5454795&Units=SI>

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
nfpaf:	NFPA Fire Rating
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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