trans-3-Methylcyclohexanol

Other names:	3-Methyl cyclohexanol, trans
	3-Methylcyclohexanol, (E)-
	Cyclohexanol, 3-methyl-, trans-
Inchi:	InChI=1S/C7H14O/c1-6-3-2-4-7(8)5-6/h6-8H,2-5H2,1H3/t6-,7-/m0/s1
InchiKey:	HTSABYAWKQAHBT-BQBZGAKWSA-N
Formula:	C7H14O
SMILES:	CC1CCCC(O)C1
Mol. weight [g/mol]:	114.19
CAS:	7443-55-2

Physical Properties

Property code	Value	Unit	Source
chl	-4356.50 ± 3.30	kJ/mol	NIST Webbook
chl	-4333.70 ± 3.30	kJ/mol	NIST Webbook
gf	-112.02	kJ/mol	Joback Method
hf	-306.06	kJ/mol	Joback Method
hfl	-421.66	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	964.00		NIST Webbook
rinpol	964.00		NIST Webbook
ripol	1459.00		NIST Webbook
ripol	1459.00		NIST Webbook
tb	466.62	K	Joback Method
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	231.22	J/mol×K	466.62	Joback Method
cpg	245.46	J/mol×K	498.70	Joback Method
cpg	259.05	J/mol×K	530.78	Joback Method
cpg	271.99	J/mol×K	562.86	Joback Method
cpg	284.31	J/mol×K	594.94	Joback Method
cpg	296.01	J/mol×K	627.01	Joback Method
cpg	307.10	J/mol×K	659.09	Joback Method
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73701e+01
Coeff. B	-4.73634e+03
Coeff. C	-6.54580e+01
Temperature range (K), min.	342.72
Temperature range (K), max.	458.23

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.46194e+01
Coeff. B	-1.02460e+04
Coeff. C	-1.10847e+01
Coeff. D	3.73987e-06
Temperature range (K), min.	272.65
Temperature range (K), max.	617.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=905
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7443552&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=905
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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