Cyclohexane, 1,2,3-trimethyl-, (1«alpha»,2«alpha»,3«beta»)-

Other names: 1,cis-2,trans-3-Trimethylcyclohexane
Cyclohexane, 1,2,3-trimethyl-, cis,trans-
Cyclohexane, 1,2,3-trimethyl-, cis-1,2,trans-1,3-
cis,trans-1,2,3-Trimethylcyclohexane

Inchi: InChI=1S/C9H18/c1-7-5-4-6-8(2)9(7)3/h7-9H,4-6H2,1-3H3/t7-,8-/m0/s1

InchiKey: DQTVJLHNWPRPPH-YUMQZZPRSA-N

Formula: C9H18

SMILES: CC1CCCC(C)C1C

Mol. weight [g/mol]: 126.24

CAS: 7667-55-2

Physical Properties

Property code	Value	Unit	Source
gf	33.93	kJ/mol	Joback Method
hf	-215.45	kJ/mol	Joback Method
hfus	13.04	kJ/mol	Joback Method
hvap	35.44	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	878.70		NIST Webbook
rinpol	885.10		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	878.35		NIST Webbook
rinpol	878.35		NIST Webbook
rinpol	897.70		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	897.70		NIST Webbook
tb	424.40 ± 0.40	K	NIST Webbook
tb	424.28 ± 0.20	K	NIST Webbook
tb	424.40	K	NIST Webbook
tc	613.57	K	Joback Method
tf	187.42 ± 0.20	K	NIST Webbook
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.82	J/mol×K	415.53	Joback Method
cpg	342.37	J/mol×K	580.57	Joback Method
cpg	326.43	J/mol×K	547.56	Joback Method
cpg	309.72	J/mol×K	514.55	Joback Method
cpg	292.21	J/mol×K	481.54	Joback Method
cpg	273.92	J/mol×K	448.54	Joback Method
cpg	357.55	J/mol×K	613.57	Joback Method
dvisc	0.0002565	Pa×s	415.53	Joback Method
dvisc	0.0003096	Pa×s	377.96	Joback Method
dvisc	0.0003896	Pa×s	340.38	Joback Method
dvisc	0.0005190	Pa×s	302.81	Joback Method
dvisc	0.0007500	Pa×s	265.24	Joback Method
dvisc	0.0012236	Pa×s	227.66	Joback Method
dvisc	0.0024227	Pa×s	190.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43748e+01
Coeff. B	-3.93828e+03
Coeff. C	-2.07410e+01
Temperature range (K), min.	300.31
Temperature range (K), max.	455.27

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7667552&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume