Cyclohexane, 1,1,3-trimethyl-

Other names:	1,1,3-TRIMETHYLCYCLOHEXANE
	CYCLOGERANIOLANE
Inchi:	InChI=1S/C9H18/c1-8-5-4-6-9(2,3)7-8/h8H,4-7H2,1-3H3
InchiKey:	PYOLJOJPIPCRDP-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CC1CCCC(C)(C)C1
Mol. weight [g/mol]:	126.24
CAS:	3073-66-3

Physical Properties

Property code	Value	Unit	Source
chl	-5882.30	kJ/mol	NIST Webbook
gf	36.15	kJ/mol	Joback Method
hf	-179.87	kJ/mol	Joback Method
hfus	5.67	kJ/mol	Joback Method
hvap	34.60	kJ/mol	Joback Method
ie	9.39	eV	NIST Webbook
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	840.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	837.80		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	839.75		NIST Webbook
rinpol	845.40		NIST Webbook
rinpol	836.50		NIST Webbook
rinpol	836.80		NIST Webbook
rinpol	850.90		NIST Webbook
rinpol	851.00		NIST Webbook

rinpol	846.00		NIST Webbook
rinpol	846.30		NIST Webbook
rinpol	847.70		NIST Webbook
rinpol	847.70		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	839.98		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	837.80		NIST Webbook
rinpol	835.50		NIST Webbook
rinpol	832.28		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	833.00		NIST Webbook
tb	409.68 ± 0.30	K	NIST Webbook
tb	411.00 ± 2.00	K	NIST Webbook
tb	410.65 ± 1.50	K	NIST Webbook
tb	411.00 ± 2.00	K	NIST Webbook
tb	410.00 ± 2.00	K	NIST Webbook
tb	412.15 ± 1.50	K	NIST Webbook
tb	409.50 ± 0.20	K	NIST Webbook
tb	409.77 ± 0.03	K	NIST Webbook
tb	410.25 ± 1.00	K	NIST Webbook
tb	409.78 ± 0.30	K	NIST Webbook
tb	409.80	K	NIST Webbook
tb	409.78	K	KDB
tc	627.99	K	Joback Method
tf	204.55 ± 0.50	K	NIST Webbook
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.95	J/mol×K	420.44	Joback Method
cpg	275.52	J/mol×K	455.03	Joback Method
cpg	293.86	J/mol×K	489.62	Joback Method
cpg	311.08	J/mol×K	524.21	Joback Method
cpg	327.25	J/mol×K	558.80	Joback Method
cpg	342.48	J/mol×K	593.40	Joback Method
cpg	356.86	J/mol×K	627.99	Joback Method
hvapt	37.70	kJ/mol	379.50	NIST Webbook
hvapt	38.60	kJ/mol	368.50	NIST Webbook
hvapt	38.40	kJ/mol	369.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37902e+01
Coeff. B	-3.24337e+03
Coeff. C	-5.63770e+01
Temperature range (K), min.	296.58
Temperature range (K), max.	438.91

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.92667e+01
Coeff. B	-7.41233e+03
Coeff. C	-9.57566e+00
Coeff. D	6.21403e-06
Temperature range (K), min.	348.15
Temperature range (K), max.	411.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3073663&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=569
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=569

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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