Cyclohexane, 1,1,2-trimethyl-

Other names: 1,1,2-Trimethylcyclohexane
Inchi: InChI=1S/C9H18/c1-8-6-4-5-7-9(8,2)3/h8H,4-7H2,1-3H3
InchiKey: MEBONNVPKOBPEA-UHFFFAOYSA-N
Formula: C9H18
SMILES: CC1CCCCC1(C)C
Mol. weight [g/mol]: 126.24
CAS: 7094-26-0

Physical Properties

Property code	Value	Unit	Source
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
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	883.00		NIST Webbook
rinpol	879.20		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	878.70		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	882.80		NIST Webbook
rinpol	879.40		NIST Webbook
rinpol	888.90		NIST Webbook
rinpol	875.66		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	846.00		NIST Webbook

rinpol	876.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	881.70		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	877.00		NIST Webbook
tb	419.14 ± 0.30	K	NIST Webbook
tb	418.25 ± 1.00	K	NIST Webbook
tb	418.40 ± 1.00	K	NIST Webbook
tb	419.15 ± 0.50	K	NIST Webbook
tc	627.99	K	Joback Method
tf	247.16 ± 4.00	K	NIST Webbook
tf	244.00 ± 0.60	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39357e+01
Coeff. B	-3.45722e+03
Coeff. C	-4.80900e+01
Temperature range (K), min.	301.40
Temperature range (K), max.	448.96

Sources

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=568
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7094260&Units=SI

Legend

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
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