1,1,4-Trimethylcyclohexane

Other names: Cyclohexane, 1,1,4-trimethyl-
Inchi: InChI=1S/C9H18/c1-8-4-6-9(2,3)7-5-8/h8H,4-7H2,1-3H3
InchiKey: UIWORXHEVNIOJG-UHFFFAOYSA-N
Formula: C9H18
SMILES: CC1CCC(C)(C)CC1
Mol. weight [g/mol]: 126.24
CAS: 7094-27-1

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	847.00		NIST Webbook
rinpol	838.90		NIST Webbook
rinpol	841.80		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	836.00		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	833.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	842.90		NIST Webbook
rinpol	837.60		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	841.00		NIST Webbook

rinpol	844.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	839.30		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	840.20		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	840.20		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	839.30		NIST Webbook
tb	408.20	K	NIST Webbook
tb	407.70 ± 0.60	K	NIST Webbook
tc	627.99	K	Joback Method
tf	218.23	K	Joback Method
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	1.40148e+01

Coeff. B	-3.42700e+03
Coeff. C	-4.34870e+01
Temperature range (K), min.	293.14
Temperature range (K), max.	437.25

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/files/research/kdb/mol/mol570.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7094271&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