Cyclohexane, 1,3,5-trimethyl-, (1«alpha»,3«alpha»,5«alpha»)-

Other names: (1«alpha»,3«alpha»,5«alpha»)-1,3,5-Trimethyl-cyclohexane
(1Â«alphaÂ»,3Â«alphaÂ»,5Â«alphaÂ»)-1,3,5-Trimethyl-cyclohexane
(Z)-1,3,5-TRIMETHYLCYCLOHEXANE
1,3,5-Trimethylcyclohexane, cis, cis
1,3,5-cis-Trimethylcyclohexane
1,3,5-trimethylcyclohexane, cis
1,CIS-3,CIS-5-TRIMETHYLCYCLOHEXANE
CIS,CIS-1,3,5-TRIMETHYLCYCLOHEXANE
Cyclohexane, 1,3,5-trimethyl-, (1«alpha»,3«alpha»,5«alpha»)-cis
Cyclohexane, 1,3,5-trimethyl-, (1Â«alphaÂ»,3Â«alphaÂ»,5Â«alphaÂ»)-cis
Cyclohexane, 1,3,5-trimethyl-, cis-
cis-1,3,5-Trimethylcyclohexane

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

InchiKey: ODNRTOSCFYDTKF-AYMMMOKOSA-N

Formula: C9H18

SMILES: CC1CC(C)CC(C)C1

Mol. weight [g/mol]: 126.24

CAS: 1795-27-3

Physical Properties

Property code	Value	Unit	Source
gf	33.93	kJ/mol	Joback Method
hf	-215.40	kJ/mol	NIST Webbook
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	864.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	848.00		NIST Webbook

rinpol	850.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	841.75		NIST Webbook
rinpol	831.30		NIST Webbook
rinpol	835.50		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	841.75		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	848.40		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	843.70		NIST Webbook
tb	412.15 ± 1.50	K	NIST Webbook
tb	411.70 ± 0.20	K	NIST Webbook
tb	411.70 ± 0.30	K	NIST Webbook
tb	411.56 ± 0.30	K	NIST Webbook
tb	412.15 ± 2.00	K	NIST Webbook
tb	411.15 ± 2.00	K	NIST Webbook
tb	411.15 ± 4.00	K	NIST Webbook
tb	411.15 ± 3.00	K	NIST Webbook
tb	411.90 ± 1.50	K	NIST Webbook
tb	412.15 ± 1.50	K	NIST Webbook
tb	412.15 ± 1.50	K	NIST Webbook
tb	223.15	K	KDB
tb	425.15 ± 6.00	K	NIST Webbook
tc	613.57	K	Joback Method
tf	223.15	K	KDB
tf	229.93 ± 0.02	K	NIST Webbook
tf	223.45 ± 0.50	K	NIST Webbook
tf	223.00 ± 5.00	K	NIST Webbook
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.55	J/mol×K	613.57	Joback Method
cpg	254.82	J/mol×K	415.53	Joback Method
cpg	273.92	J/mol×K	448.54	Joback Method
cpg	292.21	J/mol×K	481.54	Joback Method
cpg	309.72	J/mol×K	514.55	Joback Method
cpg	326.43	J/mol×K	547.56	Joback Method
cpg	342.37	J/mol×K	580.57	Joback Method
dvisc	0.0002565	Pa×s	415.53	Joback Method
dvisc	0.0024227	Pa×s	190.09	Joback Method
dvisc	0.0012236	Pa×s	227.66	Joback Method
dvisc	0.0007500	Pa×s	265.24	Joback Method
dvisc	0.0005190	Pa×s	302.81	Joback Method
dvisc	0.0003896	Pa×s	340.38	Joback Method
dvisc	0.0003096	Pa×s	377.96	Joback Method
hvapt	38.30	kJ/mol	364.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43321e+01
Coeff. B	-3.76912e+03
Coeff. C	-2.36820e+01
Temperature range (K), min.	292.05
Temperature range (K), max.	441.52

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-3.27220e+01
Coeff. B	-2.60338e+03
Coeff. C	7.48937e+00

Coeff. D	-8.61311e-06
Temperature range (K), min.	318.15
Temperature range (K), max.	607.86

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795273&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=578
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=578

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
hvapt:	Enthalpy of vaporization at a given temperature
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.