

1-Methyl-1,3-cyclohexadiene

Other names:	1,3-Cyclohexadiene, 1-methyl- 2,3-dihydrotoluene
Inchi:	InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-3,5H,4,6H2,1H3
InchiKey:	QMFJIJFIHIDENY-UHFFFAOYSA-N
Formula:	C7H10
SMILES:	CC1=CC=CCC1
Mol. weight [g/mol]:	94.15
CAS:	1489-56-1

Physical Properties

Property code	Value	Unit	Source
gf	90.51	kJ/mol	Joback Method
hf	-9.06	kJ/mol	Joback Method
hfus	6.71	kJ/mol	Joback Method
hvap	33.16	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.283		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
rinpol	791.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	771.00		NIST Webbook
tb	371.20 ± 1.00	K	NIST Webbook
tc	596.32	K	Joback Method
tf	194.31	K	Joback Method
vc	0.334	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.21	J/mol×K	387.08	Joback Method
cpg	163.02	J/mol×K	421.95	Joback Method

cpg	175.15	J/molxK	456.83	Joback Method
cpg	186.61	J/molxK	491.70	Joback Method
cpg	197.43	J/molxK	526.57	Joback Method
cpg	207.64	J/molxK	561.45	Joback Method
cpg	217.25	J/molxK	596.32	Joback Method
dvisc	0.0040402	Paxs	194.31	Joback Method
dvisc	0.0018112	Paxs	226.44	Joback Method
dvisc	0.0009911	Paxs	258.57	Joback Method
dvisc	0.0006197	Paxs	290.69	Joback Method
dvisc	0.0004254	Paxs	322.82	Joback Method
dvisc	0.0003126	Paxs	354.95	Joback Method
dvisc	0.0002418	Paxs	387.08	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43111e+01
Coeff. B	-3.16813e+03
Coeff. C	-4.43440e+01
Temperature range (K), min.	270.26
Temperature range (K), max.	396.37

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1489561&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/ci9903071

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
mccvol:	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

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