

1,3-Cyclohexadiene, 1-methyl-

Other names:	1-methyl-1,3-cyclohexadiene 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]:	94.16
CAS:	1489-56-1

Physical Properties

Property code	Value	Unit	Source
hfus	6.71	kJ/mol	Joback Method
ie	8.34	eV	Cheméo Relay (1.0)
logp	2.283		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
tb	378.97	K	Cheméo Relay (1.0)

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/mol×K	456.83	Joback Method
cpg	186.61	J/mol×K	491.70	Joback Method
cpg	197.43	J/mol×K	526.57	Joback Method
cpg	207.64	J/mol×K	561.45	Joback Method
cpg	217.25	J/mol×K	596.32	Joback Method
dvisc	0.0040402	Pa×s	194.31	Joback Method
dvisc	0.0018112	Pa×s	226.44	Joback Method
dvisc	0.0009911	Pa×s	258.57	Joback Method
dvisc	0.0006197	Pa×s	290.69	Joback Method
dvisc	0.0004254	Pa×s	322.82	Joback Method
dvisc	0.0003126	Pa×s	354.95	Joback Method
dvisc	0.0002418	Pa×s	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1489561&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

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