Dicyclopentadiene

Other names:	3A,4,7,7A-TETRAHYDRO-4,7-METHANOINDENE 3a,4,7,7a-Tetrahydro-4,7-methano-1H-indene 4,7-Methano-1H-indene, 3a,4,7,7a-tetrahydro- 4,7-Methanoindene, 3a,4,7,7a-tetrahydro- 4,7-methano-3a,4,7,7a-tetrahydro-1H-indene BICYCLOPENTADIENE Bis[cyclopentadiene] CYCLOPENTADIENE DIMER Tricyclo[5.2.1.0
Inchi:	InChI=1S/C10H12/c1-2-9-7-4-5-8(6-7)10(9)3-1/h1-2,4-5,7-10H,3,6H2/t7?,8?,9-,10+/m1/s
InchiKey:	HECLRDQVFMWTQS-BMNUFHGDSA-N
Formula:	C10H12
SMILES:	C1=CC2C3C=CC(C3)C2C1
Mol. weight [g/mol]:	132.20
CAS:	77-73-6

Physical Properties

Property code	Value	Unit	Source
gf	255.68	kJ/mol	Joback Method
hf	57.73	kJ/mol	Joback Method
hfus	17.48	kJ/mol	Joback Method
hvap	38.04	kJ/mol	Joback Method
ie	8.79 ± 0.05	eV	NIST Webbook
log10ws	-2.43		Crippen Method
logp	2.385		Crippen Method
mcvol	110.580	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	1014.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	993.30		NIST Webbook
rinpol	1018.00		NIST Webbook

rinpol	1002.00		NIST Webbook
rinpol	1004.30		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	993.30		NIST Webbook
rinpol	1047.30		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1007.00		NIST Webbook
tb	359.20 ± 50.00	K	NIST Webbook
tb	443.20	K	NIST Webbook
tc	664.47	K	Joback Method
tf	305.00 ± 4.00	K	NIST Webbook
tf	306.80 ± 0.50	K	NIST Webbook
tt	304.80 ± 0.20	K	NIST Webbook
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.89	J/mol×K	446.34	Joback Method
cpg	261.44	J/mol×K	482.70	Joback Method
cpg	278.56	J/mol×K	519.05	Joback Method
cpg	294.37	J/mol×K	555.41	Joback Method
cpg	308.96	J/mol×K	591.76	Joback Method
cpg	322.43	J/mol×K	628.12	Joback Method
cpg	334.89	J/mol×K	664.47	Joback Method
dvisc	0.0010224	Pa×s	446.34	Joback Method
dvisc	0.0005202	Pa×s	282.76	Joback Method
dvisc	0.0004087	Pa×s	250.04	Joback Method
dvisc	0.0007356	Pa×s	348.19	Joback Method
dvisc	0.0008365	Pa×s	380.91	Joback Method
dvisc	0.0009322	Pa×s	413.62	Joback Method
dvisc	0.0006298	Pa×s	315.47	Joback Method
hvapt	42.40	kJ/mol	373.50	NIST Webbook
rfi	1.50690		308.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate

rfi	1.50450	313.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.50190	318.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate
rfi	1.49910	323.15	Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-6.47025e+01
Coeff. B	-2.32780e+03
Coeff. C	1.28698e+01
Coeff. D	-1.95969e-05
Temperature range (K), min.	280.15
Temperature range (K), max.	443.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=648
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77736&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=648
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate:	https://www.doi.org/10.1021/acs.jced.6b00901

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume