

1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-

Other names: 1,3-Cyclohexadiene, 1-methyl-4-isopropyl-
1-Isopropyl-4-methyl-1,3-cyclohexadiene
1-Isopropyl-4-methyl-cyclohexa-1,3-diene
1-Methyl-4-isopropyl-1,3-cyclohexadiene
1-Methyl-4-isopropylcyclohexadiene-1,3
1-methyl-4-(1-methylethyl)-1,3-cyclohexadiene
Terpilene
alpha-Terpinene
p-Mentha-1,3-diene
«alpha»-Terpine
«alpha»-Terpinen
«alpha»-Terpinene
Â«alphaÂ»-Terpine
Â«alphaÂ»-Terpinen
Â«alphaÂ»-Terpinene

Inchi: InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,6,8H,5,7H2,1-3H3

InchiKey: YHQGMUYUVUMAZJR-UHFFFAOYSA-N

Formula: C10H16

SMILES: CC1=CC=C(C(C)C)CC1

Mol. weight [g/mol]: 136.23

CAS: 99-86-5

Physical Properties

Property code	Value	Unit	Source
chl	-5985.20	kJ/mol	NIST Webbook
gf	103.70	kJ/mol	Joback Method
hf	-87.73	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	40.11	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	1020.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1004.20		NIST Webbook

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ripol	1172.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1178.00		NIST Webbook
ripol	1189.00		NIST Webbook
ripol	1192.00		NIST Webbook
tb	447.20	K	NIST Webbook

tb	446.65 ± 0.40	K	NIST Webbook
tc	668.92	K	Joback Method
tf	225.64	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.68	J/mol×K	460.26	Joback Method
cpg	289.04	J/mol×K	495.04	Joback Method
cpg	304.56	J/mol×K	529.81	Joback Method
cpg	319.27	J/mol×K	564.59	Joback Method
cpg	333.20	J/mol×K	599.36	Joback Method
cpg	346.36	J/mol×K	634.14	Joback Method
cpg	358.80	J/mol×K	668.92	Joback Method
dvisc	0.0046457	Pa×s	225.64	Joback Method
dvisc	0.0018976	Pa×s	264.74	Joback Method
dvisc	0.0009760	Pa×s	303.85	Joback Method
dvisc	0.0005842	Pa×s	342.95	Joback Method
dvisc	0.0003884	Pa×s	382.05	Joback Method
dvisc	0.0002785	Pa×s	421.16	Joback Method
dvisc	0.0002114	Pa×s	460.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	447.70	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.36448e+01
Coeff. B	-3.44328e+03

Coeff. C	-6.57360e+01
Temperature range (K), min.	323.52
Temperature range (K), max.	478.93

Sources

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=C99865&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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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