1-Methyl-4-(1-methylethyl)-cyclohexane

Other names: 1-METHYL-4(1-METHYLETHYL)CYCLOHEXANE
1-METHYL-4-ISOPROPYLCYCLOHEXANE
1-Methyl-4-iso-propylcyclohexane,c&t
1-Methyl-4-isopropylcyclohexane (c,t)
1-isopropyl-4-methylcyclohexane
Cyclohexane, 1-methyl-4-(1-methylethyl)-
p-Menthane
para-Menthane

Inchi: InChI=1S/C10H20/c1-8(2)10-6-4-9(3)5-7-10/h8-10H,4-7H2,1-3H3

InchiKey: CFJYNSNXFXLKNS-UHFFFAOYSA-N

Formula: C10H20

SMILES: CC1CCC(C(C)C)CC1

Mol. weight [g/mol]: 140.27

CAS: 99-82-1

Physical Properties

Property code	Value	Unit	Source
gf	47.62	kJ/mol	Joback Method
hf	-221.03	kJ/mol	Joback Method
hfus	11.04	kJ/mol	Joback Method
hvap	37.59	kJ/mol	Joback Method
ie	9.32	eV	NIST Webbook
log10ws	-3.18		Crippen Method
logp	3.469		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	968.00		NIST Webbook
ripol	1122.00		NIST Webbook
tb	444.74 ± 0.40	K	NIST Webbook
tb	443.85 ± 1.00	K	NIST Webbook
tb	442.00 ± 5.00	K	NIST Webbook
tb	445.00 ± 4.00	K	NIST Webbook
tb	440.00 ± 4.00	K	NIST Webbook
tb	441.00 ± 4.00	K	NIST Webbook
tb	442.00 ± 6.00	K	NIST Webbook
tb	443.00 ± 3.00	K	NIST Webbook
tb	440.00 ± 3.00	K	NIST Webbook

tb	445.55 ± 1.50	K	NIST Webbook
tb	443.00 ± 4.00	K	NIST Webbook
tb	440.50 ± 0.50	K	NIST Webbook
tb	443.85 ± 0.50	K	NIST Webbook
tb	444.45 ± 0.50	K	NIST Webbook
tb	444.74 ± 0.40	K	NIST Webbook
tb	445.15 ± 4.00	K	NIST Webbook
tc	643.71	K	Joback Method
tf	155.15 ± 2.00	K	NIST Webbook
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.72	J/mol×K	442.64	Joback Method
cpg	320.07	J/mol×K	476.15	Joback Method
cpg	339.46	J/mol×K	509.66	Joback Method
cpg	357.93	J/mol×K	543.18	Joback Method
cpg	375.49	J/mol×K	576.69	Joback Method
cpg	392.17	J/mol×K	610.20	Joback Method
cpg	407.97	J/mol×K	643.71	Joback Method
dvisc	0.0082413	Pa×s	190.60	Joback Method
dvisc	0.0027291	Pa×s	232.61	Joback Method
dvisc	0.0012673	Pa×s	274.61	Joback Method
dvisc	0.0007213	Pa×s	316.62	Joback Method
dvisc	0.0004685	Pa×s	358.63	Joback Method
dvisc	0.0003331	Pa×s	400.63	Joback Method
dvisc	0.0002527	Pa×s	442.64	Joback Method
hvapt	43.60	kJ/mol	412.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44880e+01
Coeff. B	-3.73526e+03
Coeff. C	-6.45400e+01

Temperature range (K), min.	327.58
Temperature range (K), max.	471.59

Sources

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=588
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99821&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/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	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.