

1-Methyl-3-(1-methylethenyl)-cyclohexene

Other names:	1-Methyl-3-(1-methylethenyl)-cyclohexene
Inchi:	InChI=1S/C10H16/c1-8(2)10-6-4-5-9(3)7-10/h7,10H,1,4-6H2,2-3H3
InchiKey:	UXZIDIYMFIBDKT-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	C=C(C)C1C=C(C)CCC1
Mol. weight [g/mol]:	136.24

Physical Properties

Property code	Value	Unit	Source
hfus	11.73	kJ/mol	Joback Method
hvap	46.20	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
log10ws	-3.95		Cheméo Relay (1.0)
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
tb	449.00 ± 5.00	K	NIST Webbook
tb	451.00 ± 3.00	K	NIST Webbook
tb	448.00 ± 5.00	K	NIST Webbook
tb	450.00 ± 5.00	K	NIST Webbook
tf	194.24	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.80	J/mol×K	448.45	Joback Method
cpg	287.42	J/mol×K	483.23	Joback Method
cpg	304.13	J/mol×K	518.02	Joback Method
cpg	319.94	J/mol×K	552.80	Joback Method
cpg	334.90	J/mol×K	587.59	Joback Method
cpg	349.03	J/mol×K	622.37	Joback Method
cpg	362.36	J/mol×K	657.16	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38738602&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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