

Cyclohexene, 1,5,5-trimethyl-3-methylene-

Other names:	3-Methylene-1,5,5-trimethylcyclohexene
Inchi:	InChI=1S/C10H16/c1-8-5-9(2)7-10(3,4)6-8/h5H,1,6-7H2,2-4H3
InchiKey:	ZKXYHQFGFMZPPJ-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	<chem>C=C1C=C(C)CC(C)(C)C1</chem>
Mol. weight [g/mol]:	136.23
CAS:	16609-28-2

Physical Properties

Property code	Value	Unit	Source
affp	904.90	kJ/mol	NIST Webbook
basg	874.20	kJ/mol	NIST Webbook
gf	125.69	kJ/mol	Joback Method
hf	-49.62	kJ/mol	Joback Method
hfus	6.87	kJ/mol	Joback Method
hvap	38.25	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	451.29	K	Joback Method
tc	662.24	K	Joback Method
tf	260.70	K	Joback Method
vc	0.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.47	J/mol×K	451.29	Joback Method
cpg	289.15	J/mol×K	486.45	Joback Method
cpg	304.77	J/mol×K	521.61	Joback Method
cpg	319.42	J/mol×K	556.77	Joback Method
cpg	333.21	J/mol×K	591.93	Joback Method
cpg	346.23	J/mol×K	627.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16609282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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