1,4-Cyclohexadiene, 3,3,6,6-tetramethyl-

Other names: 3,3,6,6-Tetramethylcyclohexa-1,4-diene
Inchi: InChI=1S/C10H16/c1-9(2)5-7-10(3,4)8-6-9/h5-8H,1-4H3
InchiKey: IDFBAZYYEXBGJO-UHFFFAOYSA-N
Formula: C10H16
SMILES: CC1(C)C=CC(C)(C)C=C1
Mol. weight [g/mol]: 136.23
CAS: 2223-54-3

Physical Properties

Property code	Value	Unit	Source
gf	99.00	kJ/mol	Joback Method
hf	-69.71	kJ/mol	Joback Method
hfus	4.41	kJ/mol	Joback Method
hvap	36.26	kJ/mol	Joback Method
ie	8.81	eV	NIST Webbook
log10ws	-3.13		Crippen Method
logp	3.165		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	441.88	K	Joback Method
tc	660.85	K	Joback Method
tf	279.65 ± 2.00	K	NIST Webbook
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.18	J/mol×K	441.88	Joback Method
cpg	290.54	J/mol×K	478.37	Joback Method
cpg	307.32	J/mol×K	514.87	Joback Method
cpg	322.73	J/mol×K	551.36	Joback Method
cpg	336.98	J/mol×K	587.86	Joback Method
cpg	350.26	J/mol×K	624.35	Joback Method
cpg	362.78	J/mol×K	660.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2223543&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

Legend

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
ie:	Ionization energy
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