1,3-Cyclohexadiene, 5-methyl-

Other names: 1,3-Cyclohexadiene, 6-methyl
5-Methyl-1,3-cyclohexadiene
Inchi: InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-5,7H,6H2,1H3
InchiKey: ZNKKYYNWFKHNHZ-UHFFFAOYSA-N
Formula: C7H10
SMILES: CC1C=CC=CC1
Mol. weight [g/mol]: 94.15
CAS: 19656-98-5

Physical Properties

Property code	Value	Unit	Source
gf	92.43	kJ/mol	Joback Method
hf	-17.93	kJ/mol	Joback Method
hfus	8.16	kJ/mol	Joback Method
hvap	32.19	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.139		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	730.00		NIST Webbook
rinpol	763.00		NIST Webbook
tb	377.43	K	Joback Method
tc	584.34	K	Joback Method
tf	177.55	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.80	J/mol×K	377.43	Joback Method
cpg	162.43	J/mol×K	411.92	Joback Method
cpg	175.35	J/mol×K	446.40	Joback Method
cpg	187.58	J/mol×K	480.89	Joback Method
cpg	199.13	J/mol×K	515.37	Joback Method

cpg	210.03	J/mol×K	549.86	Joback Method
cpg	220.31	J/mol×K	584.34	Joback Method
dvisc	0.0035209	Pa×s	177.55	Joback Method
dvisc	0.0015775	Pa×s	210.86	Joback Method
dvisc	0.0008799	Pa×s	244.18	Joback Method
dvisc	0.0005646	Pa×s	277.49	Joback Method
dvisc	0.0003985	Pa×s	310.80	Joback Method
dvisc	0.0003008	Pa×s	344.12	Joback Method
dvisc	0.0002387	Pa×s	377.43	Joback Method

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=C19656985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume