

1,3-Cyclohexadiene, 5,6-dimethyl-

Inchi:	InChI=1S/C8H12/c1-7-5-3-4-6-8(7)2/h3-8H,1-2H3
InchiKey:	CJSMAFKHKCZRCX-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	CC1C=CC=CC1C
Mol. weight [g/mol]:	108.18
CAS:	5715-27-5

Physical Properties

Property code	Value	Unit	Source
gf	93.14	kJ/mol	Joback Method
hf	-58.91	kJ/mol	Joback Method
hfus	11.83	kJ/mol	Joback Method
hvap	34.11	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.385		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	395.64	K	Joback Method
tc	600.26	K	Joback Method
tf	184.58	K	Joback Method
vc	0.388	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.38	J/mol×K	395.64	Joback Method
cpg	202.57	J/mol×K	429.74	Joback Method
cpg	217.02	J/mol×K	463.85	Joback Method
cpg	230.76	J/mol×K	497.95	Joback Method
cpg	243.80	J/mol×K	532.05	Joback Method
cpg	256.15	J/mol×K	566.15	Joback Method
cpg	267.84	J/mol×K	600.26	Joback Method
dvisc	0.0020183	Paxs	184.58	Joback Method
dvisc	0.0010543	Paxs	219.76	Joback Method

dvisc	0.0006589	Paxs	254.93	Joback Method
dvisc	0.0004614	Paxs	290.11	Joback Method
dvisc	0.0003491	Paxs	325.29	Joback Method
dvisc	0.0002788	Paxs	360.46	Joback Method
dvisc	0.0002318	Paxs	395.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5715275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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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