

1,3-Cyclopentadiene, 1,2-dimethyl-

Other names:	1,2-Dimethylcyclopentadiene
Inchi:	InChI=1S/C7H10/c1-6-4-3-5-7(6)2/h3-4H,5H2,1-2H3
InchiKey:	RYILSJIMFKKICJ-UHFFFAOYSA-N
Formula:	C7H10
SMILES:	CC1=C(C)CC=C1
Mol. weight [g/mol]:	94.15
CAS:	4784-86-5

Physical Properties

Property code	Value	Unit	Source
gf	92.98	kJ/mol	Joback Method
hf	-14.37	kJ/mol	Joback Method
hfus	8.42	kJ/mol	Joback Method
hvap	33.65	kJ/mol	Joback Method
ie	8.10 ± 0.10	eV	NIST Webbook
log10ws	-2.35		Crippen Method
logp	2.283		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	387.79	K	Joback Method
tc	589.92	K	Joback Method
tf	210.35	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.95	J/molxK	387.79	Joback Method
cpg	165.29	J/molxK	421.48	Joback Method
cpg	176.05	J/molxK	455.17	Joback Method
cpg	186.25	J/molxK	488.85	Joback Method
cpg	195.92	J/molxK	522.54	Joback Method
cpg	205.07	J/molxK	556.23	Joback Method
cpg	213.74	J/molxK	589.92	Joback Method

dvisc	0.0014919	Paxs	210.35	Joback Method
dvisc	0.0009151	Paxs	239.92	Joback Method
dvisc	0.0006249	Paxs	269.50	Joback Method
dvisc	0.0004601	Paxs	299.07	Joback Method
dvisc	0.0003580	Paxs	328.64	Joback Method
dvisc	0.0002903	Paxs	358.22	Joback Method
dvisc	0.0002431	Paxs	387.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4784865&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
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

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