

1,3-Cyclopentadiene, 5-(1,1-dimethylethyl)-

Other names:	5-tert-Butyl-1,3-cyclopentadiene
Inchi:	InChI=1S/C9H14/c1-9(2,3)8-6-4-5-7-8/h4-8H,1-3H3
InchiKey:	ZATNUISQHWOHKK-UHFFFAOYSA-N
Formula:	C9H14
SMILES:	CC(C)(C)C1C=CC=C1
Mol. weight [g/mol]:	122.21
CAS:	35059-40-6

Physical Properties

Property code	Value	Unit	Source
gf	124.21	kJ/mol	Joback Method
hf	-61.80	kJ/mol	Joback Method
hfus	8.03	kJ/mol	Joback Method
hvap	35.17	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.775		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	788.00		NIST Webbook
tb	415.69	K	Joback Method
tc	624.28	K	Joback Method
tf	206.03	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.51	J/molxK	415.69	Joback Method
cpg	304.57	J/molxK	589.51	Joback Method
cpg	291.71	J/molxK	554.75	Joback Method
cpg	277.92	J/molxK	519.98	Joback Method
cpg	263.17	J/molxK	485.22	Joback Method
cpg	247.38	J/molxK	450.45	Joback Method
cpg	316.56	J/molxK	624.28	Joback Method

dvisc	0.0002993	Paxs	415.69	Joback Method
dvisc	0.0003830	Paxs	380.75	Joback Method
dvisc	0.0005153	Paxs	345.80	Joback Method
dvisc	0.0007411	Paxs	310.86	Joback Method
dvisc	0.0011685	Paxs	275.92	Joback Method
dvisc	0.0021026	Paxs	240.97	Joback Method
dvisc	0.0046178	Paxs	206.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35059406&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
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

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