

1,3-Cyclopentadiene, 1-(2-methylpropyl)

Inchi:	InChI=1S/C9H14/c1-8(2)7-9-5-3-4-6-9/h3-5,8H,6-7H2,1-2H3
InchiKey:	GHJATKVLNMETBA-UHFFFAOYSA-N
Formula:	C9H14
SMILES:	CC(C)CC1=CC=CC1
Mol. weight [g/mol]:	122.21

Physical Properties

Property code	Value	Unit	Source
gf	117.01	kJ/mol	Joback Method
hf	-49.46	kJ/mol	Joback Method
hfus	10.46	kJ/mol	Joback Method
hvap	37.05	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.919		Crippen Method
mvol	118.210	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	867.00		NIST Webbook
ripol	1052.10		NIST Webbook
tb	428.13	K	Joback Method
tc	629.76	K	Joback Method
tf	205.37	K	Joback Method
vc	0.448	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.97	J/molxK	428.13	Joback Method
cpg	244.79	J/molxK	461.73	Joback Method
cpg	258.79	J/molxK	495.34	Joback Method
cpg	272.03	J/molxK	528.94	Joback Method
cpg	284.53	J/molxK	562.55	Joback Method
cpg	296.33	J/molxK	596.15	Joback Method
cpg	307.45	J/molxK	629.76	Joback Method
dvisc	0.0044006	Paxs	205.37	Joback Method

dvisc	0.0019215	Paxs	242.50	Joback Method
dvisc	0.0010455	Paxs	279.62	Joback Method
dvisc	0.0006561	Paxs	316.75	Joback Method
dvisc	0.0004541	Paxs	353.88	Joback Method
dvisc	0.0003370	Paxs	391.00	Joback Method
dvisc	0.0002633	Paxs	428.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R40685&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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