

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

Other names:	1,3-Cyclopentadiene, 5-sec-butylidene-Cyclopentadiene, 5-sec-butylidene-Fulvene, 6-ethyl-6-methyl-6-Ethyl-6-methylfulvene 6-Methyl-6-ethylfulvene
Inchi:	InChI=1S/C9H12/c1-3-8(2)9-6-4-5-7-9/h4-7H,3H2,1-2H3
InchiKey:	HRYYXFYLNRICQD-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	CCC(C)=C1C=CC=C1
Mol. weight [g/mol]:	120.19
CAS:	3141-02-4

Physical Properties

Property code	Value	Unit	Source
gf	165.99	kJ/mol	Joback Method
hf	33.53	kJ/mol	Joback Method
hfus	13.39	kJ/mol	Joback Method
hvap	37.65	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.839		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	430.11	K	Joback Method
tc	637.22	K	Joback Method
tf	204.25	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.16	J/molxK	430.11	Joback Method
cpg	229.00	J/molxK	464.63	Joback Method
cpg	242.01	J/molxK	499.15	Joback Method
cpg	254.22	J/molxK	533.67	Joback Method

cpg	265.68	J/mol×K	568.18	Joback Method
cpg	276.44	J/mol×K	602.70	Joback Method
cpg	286.54	J/mol×K	637.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3141024&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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