1,3-Cyclopentadiene, 1,2,5,5-tetramethyl-

Other names: 1,2,5,5-Tetramethyl-1,3-cyclopentadiene
Inchi: InChI=1S/C9H14/c1-7-5-6-9(3,4)8(7)2/h5-6H,1-4H3
InchiKey: FZQSOBIGZJECPN-UHFFFAOYSA-N
Formula: C9H14
SMILES: CC1=C(C)C(C)(C)C=C1
Mol. weight [g/mol]: 122.21
CAS: 4249-12-1

Physical Properties

Property code	Value	Unit	Source
gf	96.62	kJ/mol	Joback Method
hf	-60.75	kJ/mol	Joback Method
hfus	8.37	kJ/mol	Joback Method
hvap	36.64	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.919		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	834.70		NIST Webbook
rinpol	834.70		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	840.00		NIST Webbook
tb	429.12	K	Joback Method
tc	635.97	K	Joback Method
tf	252.55	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.64	J/mol×K	429.12	Joback Method
cpg	247.23	J/mol×K	463.59	Joback Method
cpg	260.83	J/mol×K	498.07	Joback Method
cpg	273.51	J/mol×K	532.54	Joback Method

cpg	285.39	J/mol×K	567.02	Joback Method
cpg	296.56	J/mol×K	601.49	Joback Method
cpg	307.11	J/mol×K	635.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4249121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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