

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:	<chem>CC1=C(C)C(C)(C)C=C1</chem>
Mol. weight [g/mol]:	122.21

Physical Properties

Property code	Value	Unit	Source
hfus	8.37	kJ/mol	Joback Method
logp	2.919		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
rinpol	834.70		NIST Webbook
rinpol	834.70		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	840.00		NIST Webbook

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4249121&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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