

1,3-Cyclohexadiene, 1,2,6,6-tetramethyl-

Other names:	«beta»-Pyronene 1,2,6,6-Tetramethyl-1,3-Cyclohexadiene
Inchi:	InChI=1S/C10H16/c1-8-6-5-7-10(3,4)9(8)2/h5-6H,7H2,1-4H3
InchiKey:	RSTKTCUSOWRUNR-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	CC1=C(C)C(C)(C)CC=C1
Mol. weight [g/mol]:	136.23
CAS:	514-96-5

Physical Properties

Property code	Value	Unit	Source
gf	92.94	kJ/mol	Joback Method
hf	-87.55	kJ/mol	Joback Method
hfus	8.86	kJ/mol	Joback Method
hvap	39.04	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	999.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	993.00		NIST Webbook
tb	456.27	K	Joback Method
tc	668.83	K	Joback Method
tf	260.30	K	Joback Method
vc	0.498	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.78	J/mol×K	456.27	Joback Method
cpg	290.27	J/mol×K	491.70	Joback Method

cpg	305.70	J/mol×K	527.12	Joback Method
cpg	320.17	J/mol×K	562.55	Joback Method
cpg	333.78	J/mol×K	597.98	Joback Method
cpg	346.62	J/mol×K	633.40	Joback Method
cpg	358.81	J/mol×K	668.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C514965&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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