1,3-Cyclohexadiene, 1,5,5,6-tetramethyl-

Other names: «alpha»-Pyronene
1,5,5,6-tetramethyl-1,3-cyclohexadiene
Inchi: InChI=1S/C10H16/c1-8-6-5-7-10(3,4)9(8)2/h5-7,9H,1-4H3
InchiKey: LKNRSUKTEIJIAS-UHFFFAOYSA-N
Formula: C10H16
SMILES: CC1=CC=CC(C)(C)C1C
Mol. weight [g/mol]: 136.23
CAS: 514-94-3

Physical Properties

Property code	Value	Unit	Source
gf	94.86	kJ/mol	Joback Method
hf	-96.42	kJ/mol	Joback Method
hfus	10.32	kJ/mol	Joback Method
hvap	38.07	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.165		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
ripol	1365.00		NIST Webbook
tb	446.62	K	Joback Method
tc	657.46	K	Joback Method
tf	243.54	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.86	J/mol×K	446.62	Joback Method
cpg	290.23	J/mol×K	481.76	Joback Method
cpg	306.48	J/mol×K	516.90	Joback Method
cpg	321.73	J/mol×K	552.04	Joback Method
cpg	336.05	J/mol×K	587.18	Joback Method
cpg	349.55	J/mol×K	622.32	Joback Method

cpg	362.33	J/mol×K	657.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C514943&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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