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

Other names:	1,3-Cyclopentadiene, 5-isopropylidene- Dimethylfulvene Isopropylidenecyclopentadiene 5-Isopropylidene-1,3-cyclopentadiene 6,6-Dimethylfulvene 5-(1-Methylethylidene)-1,3-cyclopentadiene 5-Isopropylidenecyclopentadiene Fulvene, 6,6-dimethyl
Inchi:	InChI=1S/C8H10/c1-7(2)8-5-3-4-6-8/h3-6H,1-2H3
InchiKey:	WXACXMWYHXOSIX-UHFFFAOYSA-N
Formula:	C8H10
SMILES:	CC(C)=C1C=CC=C1
Mol. weight [g/mol]:	106.17
CAS:	2175-91-9

Physical Properties

Property code	Value	Unit	Source
chl	-4667.30 ± 5.00	kJ/mol	NIST Webbook
gf	157.57	kJ/mol	Joback Method
hf	144.00	kJ/mol	NIST Webbook
hfus	10.80	kJ/mol	Joback Method
hvap	44.18	kJ/mol	NIST Webbook
ie	8.03	eV	NIST Webbook
log10ws	-2.63		Crippen Method
logp	2.449		Crippen Method
mcvol	99.820	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
rinpol	858.00		NIST Webbook
ripol	1170.00		NIST Webbook
tb	407.23	K	Joback Method
tc	616.65	K	Joback Method
tf	274.05 ± 2.00	K	NIST Webbook
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.95	J/mol×K	407.23	Joback Method
cpg	188.59	J/mol×K	442.13	Joback Method
cpg	200.45	J/mol×K	477.04	Joback Method
cpg	211.56	J/mol×K	511.94	Joback Method
cpg	221.96	J/mol×K	546.85	Joback Method
cpg	231.70	J/mol×K	581.75	Joback Method
cpg	240.82	J/mol×K	616.65	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.70	K	6.70	NIST Webbook
tbrp	332.50 ± 0.50	K	3.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2175919&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

chl: Standard liquid enthalpy of combustion
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

ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume