Cyclopentadienyl radical

Inchi: InChI=1S/C5H5/c1-2-4-5-3-1/h1-5H
InchiKey: HPYIUKIBUJFXII-UHFFFAOYSA-N
Formula: C5H5
SMILES: [CH]1C=CC=C1
Mol. weight [g/mol]: 65.09
CAS: 2143-53-5

Physical Properties

Property code	Value	Unit	Source
affp	831.50	kJ/mol	NIST Webbook
basg	799.10	kJ/mol	NIST Webbook
ea	1.79 ± 0.05	eV	NIST Webbook
ea	1.93 ± 0.13	eV	NIST Webbook
ea	1.84 ± 0.03	eV	NIST Webbook
ea	2.20 ± 0.30	eV	NIST Webbook
ea	1.79 ± 0.02	eV	NIST Webbook
gf	140.07	kJ/mol	Joback Method
hf	85.32	kJ/mol	Joback Method
hfus	6.77	kJ/mol	Joback Method
hvap	27.42	kJ/mol	Joback Method
ie	8.41	eV	NIST Webbook
ie	8.56	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-1.13		Crippen Method
logp	1.317		Crippen Method
mcvol	59.700	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	326.70	K	Joback Method
tc	522.39	K	Joback Method
tf	174.90	K	Joback Method
vc	0.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	77.18	J/mol×K	326.70	Joback Method
cpg	86.69	J/mol×K	359.31	Joback Method
cpg	95.48	J/mol×K	391.93	Joback Method
cpg	103.59	J/mol×K	424.54	Joback Method
cpg	111.08	J/mol×K	457.16	Joback Method
cpg	117.97	J/mol×K	489.77	Joback Method
cpg	124.32	J/mol×K	522.39	Joback Method
dvisc	0.0002442	Pa×s	174.90	Joback Method
dvisc	0.0002362	Pa×s	200.20	Joback Method
dvisc	0.0002301	Pa×s	225.50	Joback Method
dvisc	0.0002254	Pa×s	250.80	Joback Method
dvisc	0.0002216	Pa×s	276.10	Joback Method
dvisc	0.0002185	Pa×s	301.40	Joback Method
dvisc	0.0002159	Pa×s	326.70	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2143535&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
ea: Electron affinity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume