2-Methyl-1,3-cyclopentadiene

Other names:	1,3-Cyclopentadiene,2-methyl- Cyclopentadiene, 2-methyl Cyclopentadiene, 3-methyl
Inchi:	InChI=1S/C6H8/c1-6-4-2-3-5-6/h2,4-5H,3H2,1H3
InchiKey:	AHQZRFBZJSCKAV-UHFFFAOYSA-N
Formula:	C6H8
SMILES:	CC1=CCC=C1
Mol. weight [g/mol]:	80.13
CAS:	3727-31-9

Physical Properties

Property code	Value	Unit	Source
gf	94.19	kJ/mol	Joback Method
hf	17.74	kJ/mol	Joback Method
hfus	6.22	kJ/mol	Joback Method
hvap	30.76	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.46 ± 0.05	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
log10ws	-1.94		Crippen Method
logp	1.893		Crippen Method
mcvol	75.940	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
rinpol	642.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	627.50		NIST Webbook
rinpol	653.80		NIST Webbook
rinpol	649.60		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	622.80		NIST Webbook
rinpol	631.00		NIST Webbook

rinpol	621.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	644.00		NIST Webbook
ripol	834.20		NIST Webbook
tb	359.93	K	Joback Method
tc	561.67	K	Joback Method
tf	186.56	K	Joback Method
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.91	J/mol×K	359.93	Joback Method
cpg	163.69	J/mol×K	528.04	Joback Method
cpg	155.42	J/mol×K	494.42	Joback Method
cpg	146.63	J/mol×K	460.80	Joback Method
cpg	137.29	J/mol×K	427.18	Joback Method
cpg	127.40	J/mol×K	393.55	Joback Method
cpg	171.48	J/mol×K	561.67	Joback Method
dvisc	0.0002409	Pa×s	359.93	Joback Method
dvisc	0.0002919	Pa×s	331.03	Joback Method
dvisc	0.0003668	Pa×s	302.14	Joback Method
dvisc	0.0004838	Pa×s	273.25	Joback Method
dvisc	0.0006814	Pa×s	244.35	Joback Method
dvisc	0.0010520	Pa×s	215.45	Joback Method
dvisc	0.0018579	Pa×s	186.56	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=C3727319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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