1,3-Cyclopentadiene, 5-methyl-

Other names: 5-Methyl-1,3-cyclopentadiene
5-Methylcyclopentadiene
Inchi: InChI=1S/C6H8/c1-6-4-2-3-5-6/h2-6H,1H3
InchiKey: QVRBGKYLLCLCHL-UHFFFAOYSA-N
Formula: C6H8
SMILES: CC1C=CC=C1
Mol. weight [g/mol]: 80.13
CAS: 96-38-8

Physical Properties

Property code	Value	Unit	Source
gf	96.11	kJ/mol	Joback Method
hf	8.87	kJ/mol	Joback Method
hfus	7.67	kJ/mol	Joback Method
hvap	29.79	kJ/mol	Joback Method
ie	8.45 ± 0.02	eV	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.748		Crippen Method
mcvol	75.940	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
rinpol	639.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	645.00		NIST Webbook
ripol	870.40		NIST Webbook
ripol	870.40		NIST Webbook
tb	350.28	K	Joback Method
tc	549.43	K	Joback Method
tf	169.80	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.42	J/mol×K	350.28	Joback Method
cpg	126.71	J/mol×K	383.47	Joback Method
cpg	137.39	J/mol×K	416.66	Joback Method
cpg	147.48	J/mol×K	449.85	Joback Method
cpg	156.99	J/mol×K	483.04	Joback Method
cpg	165.96	J/mol×K	516.23	Joback Method
cpg	174.41	J/mol×K	549.43	Joback Method
dvisc	0.0013719	Pa×s	169.80	Joback Method
dvisc	0.0008098	Pa×s	199.88	Joback Method
dvisc	0.0005487	Pa×s	229.96	Joback Method
dvisc	0.0004068	Pa×s	260.04	Joback Method
dvisc	0.0003209	Pa×s	290.12	Joback Method
dvisc	0.0002647	Pa×s	320.20	Joback Method
dvisc	0.0002257	Pa×s	350.28	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=C96388&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