Benzene, (1-methyl-2-cyclopropen-1-yl)-

Other names: 3-Methyl-3-phenylcyclopropene
1-Cyclopropene, 3-methyl-3-phenyl-
1-Methyl-1-phenyl-2-cyclopropene
Inchi: InChI=1S/C10H10/c1-10(7-8-10)9-5-3-2-4-6-9/h2-8H,1H3
InchiKey: QPQKDBYTARBUDX-UHFFFAOYSA-N
Formula: C10H10
SMILES: CC1(c2ccccc2)C=C1
Mol. weight [g/mol]: 130.19
CAS: 65051-83-4

Physical Properties

Property code	Value	Unit	Source
gf	230.95	kJ/mol	Joback Method
hf	132.62	kJ/mol	Joback Method
hfus	8.76	kJ/mol	Joback Method
hvap	39.18	kJ/mol	Joback Method
ie	8.49	eV	NIST Webbook
ie	8.29	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-2.53		Crippen Method
logp	2.514		Crippen Method
mcvol	112.840	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	461.02	K	Joback Method
tc	695.62	K	Joback Method
tf	271.48	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.03	J/mol×K	461.02	Joback Method
cpg	242.32	J/mol×K	500.12	Joback Method
cpg	256.12	J/mol×K	539.22	Joback Method

cpg	268.62	J/mol×K	578.32	Joback Method
cpg	280.00	J/mol×K	617.42	Joback Method
cpg	290.47	J/mol×K	656.52	Joback Method
cpg	300.20	J/mol×K	695.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65051834&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

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
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