Benzene,1-methyl-1,2-propadienyl-

Other names: 1,2-Butadiene, 3-phenyl-
Inchi: InChI=1S/C10H10/c1-3-9(2)10-7-5-4-6-8-10/h4-8H,1H2,2H3
InchiKey: IHOYDALOVDQINJ-UHFFFAOYSA-N
Formula: C10H10
SMILES: C=C=C(C)c1ccccc1
Mol. weight [g/mol]: 130.19
CAS: 22433-39-2

Physical Properties

Property code	Value	Unit	Source
gf	353.30	kJ/mol	Joback Method
hf	265.22	kJ/mol	Joback Method
hfus	15.24	kJ/mol	Joback Method
hvap	39.98	kJ/mol	Joback Method
ie	8.07	eV	NIST Webbook
log10ws	-3.01		Crippen Method
logp	2.875		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	454.71	K	Joback Method
tc	682.08	K	Joback Method
tf	219.67	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.10	J/mol×K	454.71	Joback Method
cpg	240.97	J/mol×K	492.61	Joback Method
cpg	254.01	J/mol×K	530.50	Joback Method
cpg	266.26	J/mol×K	568.40	Joback Method
cpg	277.74	J/mol×K	606.29	Joback Method
cpg	288.48	J/mol×K	644.19	Joback Method
cpg	298.52	J/mol×K	682.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22433392&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