Benzene,[2-methyl-3-(2-methyl-1-propenylidene)c

Inchi: InChI=1S/C14H16/c1-10(2)9-13-11(3)14(13)12-7-5-4-6-8-12/h4-8,11,14H,1-3H3/t11-,14+
InchiKey: WBZZBXVCSQAKIK-RISCZKNCSA-N
Formula: C14H16
SMILES: CC(C)=C=C1C(C)C1c1ccccc1
Mol. weight [g/mol]: 184.28
CAS: 33530-26-6

Physical Properties

Property code	Value	Unit	Source
gf	397.64	kJ/mol	Joback Method
hf	185.72	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
ie	7.65	eV	NIST Webbook
log10ws	-4.13		Crippen Method
logp	3.911		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	558.26	K	Joback Method
tc	790.01	K	Joback Method
tf	290.57	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.28	J/mol×K	558.26	Joback Method
cpg	412.76	J/mol×K	596.89	Joback Method
cpg	430.03	J/mol×K	635.51	Joback Method
cpg	446.17	J/mol×K	674.14	Joback Method
cpg	461.23	J/mol×K	712.76	Joback Method
cpg	475.28	J/mol×K	751.39	Joback Method
cpg	488.39	J/mol×K	790.01	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=C33530266&Units=SI

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