Benzene, 1,2-propadienyl-

Other names:	Benzene, propadienyl-
	Phenylallene
	Phenylpropadiene
	1,2-Propadiene, 1-phenyl-
Inchi:	InChI=1S/C9H8/c1-2-6-9-7-4-3-5-8-9/h3-8H,1H2
InchiKey:	WEHMXWJFCCNXHJ-UHFFFAOYSA-N
Formula:	C9H8
SMILES:	C=C=Cc1ccccc1
Mol. weight [g/mol]:	116.16
CAS:	2327-99-3

Physical Properties

Property code	Value	Unit	Source
gf	353.43	kJ/mol	Joback Method
hf	295.65	kJ/mol	Joback Method
hfus	13.96	kJ/mol	Joback Method
hvap	37.67	kJ/mol	Joback Method
ie	8.29	eV	NIST Webbook
log10ws	-2.59		Crippen Method
logp	2.485		Crippen Method
mcvol	105.310	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
tb	431.95	K	Joback Method
tc	657.97	K	Joback Method
tf	222.36	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.44	J/mol×K	431.95	Joback Method
cpg	199.77	J/mol×K	469.62	Joback Method
cpg	211.37	J/mol×K	507.29	Joback Method
cpg	222.27	J/mol×K	544.96	Joback Method

cpg	232.50	J/mol×K	582.63	Joback Method
cpg	242.06	J/mol×K	620.30	Joback Method
cpg	251.00	J/mol×K	657.97	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=C2327993&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