Benzene, (1-methylene-2-propenyl)-

Other names:	1,3-Butadiene, 2-phenyl-
	Phenoprene
	2-Phenylbutadiene
	2-Phenyl-1,3-butadiene
Inchi:	InChI=1S/C10H10/c1-3-9(2)10-7-5-4-6-8-10/h3-8H,1-2H2
InchiKey:	IMJGQTCMUZMLRZ-UHFFFAOYSA-N
Formula:	C10H10
SMILES:	C=CC(=C)c1ccccc1
Mol. weight [g/mol]:	130.19
CAS:	2288-18-8

Physical Properties

Property code	Value	Unit	Source
gf	312.86	kJ/mol	Joback Method
hf	227.87	kJ/mol	Joback Method
hfus	11.83	kJ/mol	Joback Method
hvap	38.87	kJ/mol	Joback Method
ie	8.57	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.10 ± 0.05	eV	NIST Webbook
ie	8.19	eV	NIST Webbook
log10ws	-2.99		Crippen Method
logp	2.886		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	1140.20		NIST Webbook
tb	448.12	K	Joback Method
tc	666.44	K	Joback Method
tf	211.40	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	223.21	J/mol×K	448.12	Joback Method
cpg	237.28	J/mol×K	484.51	Joback Method
cpg	250.41	J/mol×K	520.89	Joback Method
cpg	262.66	J/mol×K	557.28	Joback Method
cpg	274.07	J/mol×K	593.67	Joback Method
cpg	284.70	J/mol×K	630.06	Joback Method
cpg	294.59	J/mol×K	666.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.70	K	2.30	NIST Webbook

Sources

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=C2288188&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume