(Z)-1-Phenylpropene

Other names:	(Z)-1-Propenylbenzene
	1-Phenyl-1-propene, cis-
	Benzene, (1Z)-1-propenyl-
	Benzene, 1-propenyl-, (Z)-
	Benzene, propen-1-yl-, (Z)-
	Benzene, propenyl-, (Z)-
	cis-1-Phenyl-1-propene
	cis-1-Phenylpropene
	cis-1-Propenylbenzene
	cis-Propenylbenzene
	cis-«beta»-Methylstyrene
	cis-Â«betaÂ»-Methylstyrene
Inchi:	InChI=1S/C9H10/c1-2-6-9-7-4-3-5-8-9/h2-8H,1H3/b6-2-
InchiKey:	QROGIFZRVHSFLM-KXFIGUGUSA-N
Formula:	C9H10
SMILES:	CC=Cc1ccccc1
Mol. weight [g/mol]:	118.18
CAS:	766-90-5

Physical Properties

Property code	Value	Unit	Source
affp	836.40	kJ/mol	NIST Webbook
basg	807.50	kJ/mol	NIST Webbook
chg	-5092.14	kJ/mol	NIST Webbook
gf	217.53	kJ/mol	Joback Method
hf	124.66	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	37.86	kJ/mol	Joback Method
ie	8.48	eV	NIST Webbook
ie	8.15	eV	NIST Webbook
ie	8.15	eV	NIST Webbook
ie	8.28	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
log10ws	-2.71		Crippen Method
logp	2.720		Crippen Method
mcvol	109.610	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method

rinpol	975.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	155.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	155.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	975.30		NIST Webbook
ripol	1324.30		NIST Webbook
ripol	1324.00		NIST Webbook
tb	441.65 ± 3.00	K	NIST Webbook
tb	440.58 ± 0.30	K	NIST Webbook
tc	654.10	K	Joback Method
tf	211.23 ± 0.20	K	NIST Webbook
tf	203.40 ± 1.00	K	NIST Webbook
tf	211.47 ± 0.15	K	NIST Webbook
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.03	J/mol×K	436.16	Joback Method
cpg	212.72	J/mol×K	472.48	Joback Method
cpg	225.50	J/mol×K	508.81	Joback Method
cpg	237.43	J/mol×K	545.13	Joback Method
cpg	248.56	J/mol×K	581.46	Joback Method
cpg	258.93	J/mol×K	617.78	Joback Method
cpg	268.59	J/mol×K	654.10	Joback Method
dvisc	0.0032236	Pa×s	212.53	Joback Method
dvisc	0.0014202	Pa×s	249.80	Joback Method
dvisc	0.0007741	Pa×s	287.07	Joback Method
dvisc	0.0004851	Pa×s	324.34	Joback Method
dvisc	0.0003347	Pa×s	361.62	Joback Method
dvisc	0.0002476	Pa×s	398.89	Joback Method
dvisc	0.0001928	Pa×s	436.16	Joback Method
hvapt	44.80	kJ/mol	423.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56145e+01
Coeff. B	-4.32144e+03
Coeff. C	-4.75840e+01
Temperature range (K), min.	329.54
Temperature range (K), max.	467.02

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C766905&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume