Benzene, 2-propenyl-

Other names:	1-Phenyl-2-propene
	1-Propene, 3-phenyl-
	2-Propenylbenzene
	3-Phenyl-1-propene
	3-Phenylpropene
	Allylbenzene
	Benzene, allyl-
Inchi:	InChI=1S/C9H10/c1-2-6-9-7-4-3-5-8-9/h2-5,7-8H,1,6H2
InchiKey:	HJWLCRVIBGQPNF-UHFFFAOYSA-N
Formula:	C9H10
SMILES:	C=CCc1ccccc1
Mol. weight [g/mol]:	118.18
CAS:	300-57-2

Physical Properties

Property code	Value	Unit	Source
chl	-5169.30	kJ/mol	NIST Webbook
gf	225.15	kJ/mol	Joback Method
hf	132.87	kJ/mol	Joback Method
hfus	11.83	kJ/mol	Joback Method
hvap	46.30 ± 0.20	kJ/mol	NIST Webbook
ie	8.20 ± 0.02	eV	NIST Webbook
ie	9.16	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	7.80 ± 0.10	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.415		Crippen Method
mcvol	109.610	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	934.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	154.50		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	914.00		NIST Webbook

rinpol	927.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	932.60		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	143.10		NIST Webbook
rinpol	917.80		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	938.90		NIST Webbook
rinpol	943.60		NIST Webbook
rinpol	950.50		NIST Webbook
rinpol	917.80		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	929.30		NIST Webbook
rinpol	929.30		NIST Webbook
rinpol	929.30		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	951.50		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	934.40		NIST Webbook
rinpol	934.40		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	930.00		NIST Webbook
ripol	1240.00		NIST Webbook
ripol	1240.00		NIST Webbook
ripol	1291.10		NIST Webbook
ripol	1263.20		NIST Webbook
ripol	1263.00		NIST Webbook
tb	428.68	K	Joback Method
tc	640.52	K	Joback Method
tf	233.15 ± 4.00	K	NIST Webbook
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.96	J/mol×K	428.68	Joback Method

cpg	212.33	J/mol×K	463.99	Joback Method
cpg	224.89	J/mol×K	499.29	Joback Method
cpg	236.67	J/mol×K	534.60	Joback Method
cpg	247.71	J/mol×K	569.90	Joback Method
cpg	258.05	J/mol×K	605.21	Joback Method
cpg	267.72	J/mol×K	640.52	Joback Method
dvisc	0.0030563	Pa×s	215.85	Joback Method
dvisc	0.0014635	Pa×s	251.32	Joback Method
dvisc	0.0008408	Pa×s	286.79	Joback Method
dvisc	0.0005458	Pa×s	322.26	Joback Method
dvisc	0.0003859	Pa×s	357.74	Joback Method
dvisc	0.0002905	Pa×s	393.21	Joback Method
dvisc	0.0002292	Pa×s	428.68	Joback Method
hvapt	46.50 ± 0.20	kJ/mol	293.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43101e+01
Coeff. B	-3.57239e+03
Coeff. C	-6.03980e+01
Temperature range (K), min.	315.16
Temperature range (K), max.	457.39

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

Diffusion coefficients of 2-fluoroanisole, 2-bromoanisole, divinylbenzene and 1,3-divinylbenzene at infinite dilution in supercritical carbon dioxide: https://www.doi.org/10.1016/j.fluid.2007.07.039

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=C300572&Units=SI

Legend

chl:	Standard liquid 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