Benzene, 1-propenyl-

Other names:	1-Phenyl-1-propene
	1-Phenylpropene
	1-Propene, 1-phenyl-
	1-Propenylbenzene
	Benzene, propenyl-
	Isoallylbenzene
	NSC 65591
	Propenylbenzene
	«beta»-Methylstyrene
	«beta»-Methylstyrol
	«omega»-Methylstyrene
	Â«betaÂ»-Methylstyrene
	Â«betaÂ»-Methylstyrol
	Â«omegaÂ»-Methylstyrene
Inchi:	InChI=1S/C9H10/c1-2-6-9-7-4-3-5-8-9/h2-8H,1H3
InchiKey:	QROGIFZRVHSFLM-UHFFFAOYSA-N
Formula:	C9H10
SMILES:	CC=Cc1ccccc1
Mol. weight [g/mol]:	118.18
CAS:	637-50-3

Physical Properties

Property code	Value	Unit	Source
chl	-4797.00	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	8.50 ± 0.10	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	1004.20		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	166.50		NIST Webbook
rinpol	165.63		NIST Webbook

rinpol	1011.20		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1004.20		NIST Webbook
rinpol	1004.20		NIST Webbook
rinpol	1004.20		NIST Webbook
rinpol	1004.20		NIST Webbook
rinpol	1004.20		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1015.90		NIST Webbook
rinpol	1011.20		NIST Webbook
rinpol	1026.00		NIST Webbook
tb	450.00 ± 3.00	K	NIST Webbook
tb	446.15 ± 3.00	K	NIST Webbook
tb	447.15 ± 2.00	K	NIST Webbook
tb	448.65 ± 1.50	K	NIST Webbook
tb	446.15 ± 2.00	K	NIST Webbook
tb	445.15 ± 5.00	K	NIST Webbook
tb	448.15 ± 2.00	K	NIST Webbook
tb	447.65 ± 3.00	K	NIST Webbook
tb	447.65 ± 1.50	K	NIST Webbook
tc	654.10	K	Joback Method
tf	212.53	K	Joback Method
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45067e+01
Coeff. B	-3.76870e+03
Coeff. C	-6.58750e+01
Temperature range (K), min.	330.92
Temperature range (K), max.	475.73

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=C637503&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume