Benzene, 3-butenyl-

Other names:	1-Butene, 4-phenyl-
	1-Phenyl-3-butene
	3-Butenylbenzene
	4-Phenyl-1-butene
	4-Phenylbut-1-ene
	4-Phenylbutene-1
Inchi:	InChI=1S/C10H12/c1-2-3-7-10-8-5-4-6-9-10/h2,4-6,8-9H,1,3,7H2
InchiKey:	PBGVMIDTGGTBFS-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	C=CCCc1ccccc1
Mol. weight [g/mol]:	132.20
CAS:	768-56-9

Physical Properties

Property code	Value	Unit	Source
chl	-5683.50	kJ/mol	NIST Webbook
gf	233.57	kJ/mol	Joback Method
hf	112.23	kJ/mol	Joback Method
hfl	7.90	kJ/mol	NIST Webbook
hfl	33.40 ± 5.00	kJ/mol	NIST Webbook
hfus	14.42	kJ/mol	Joback Method
hvap	39.46	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.83	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	2.805		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1022.00		NIST Webbook
tb	454.25 ± 0.50	K	NIST Webbook
tb	450.20	K	NIST Webbook
tb	452.00 ± 3.00	K	NIST Webbook
tb	449.15 ± 2.00	K	NIST Webbook
tb	454.70 ± 0.50	K	NIST Webbook

tb	450.15 ± 2.00	K	NIST Webbook
tb	448.15 ± 6.00	K	NIST Webbook
tc	660.72	K	Joback Method
tf	227.12	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.71	J/mol×K	451.56	Joback Method
cpg	254.20	J/mol×K	486.42	Joback Method
cpg	267.83	J/mol×K	521.28	Joback Method
cpg	280.64	J/mol×K	556.14	Joback Method
cpg	292.66	J/mol×K	591.00	Joback Method
cpg	303.94	J/mol×K	625.86	Joback Method
cpg	314.51	J/mol×K	660.72	Joback Method
dvisc	0.0032741	Pa×s	227.12	Joback Method
dvisc	0.0015315	Pa×s	264.53	Joback Method
dvisc	0.0008648	Pa×s	301.93	Joback Method
dvisc	0.0005539	Pa×s	339.34	Joback Method
dvisc	0.0003876	Pa×s	376.75	Joback Method
dvisc	0.0002893	Pa×s	414.15	Joback Method
dvisc	0.0002266	Pa×s	451.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43023e+01

Coeff. B	-3.72551e+03
Coeff. C	-6.62920e+01
Temperature range (K), min.	332.12
Temperature range (K), max.	480.66

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C768569&Units=SI
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

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

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