

Benzene, (1-methyl-1-propenyl)-, (E)-

Other names:	2-Butene, 2-phenyl-, (E)- (E)-2-Phenyl-2-butene trans-2-Phenyl-2-butene 2-Butene, 2-phenyl-, trans (E)-(1-Methylpropenyl)benzene (E)-(1-Methyl-1-propenyl)benzene Benzene, ((1E)-1-methyl-1-propenyl)-
Inchi:	InChI=1S/C10H12/c1-3-9(2)10-7-5-4-6-8-10/h3-8H,1-2H3/b9-3+
InchiKey:	UGUYQBMBIJFNRM-YCRREMRBSA-N
Formula:	C10H12
SMILES:	CC=C(C)c1ccccc1
Mol. weight [g/mol]:	132.20
CAS:	768-00-3

Physical Properties

Property code	Value	Unit	Source
chl	-5746.30	kJ/mol	NIST Webbook
gf	217.40	kJ/mol	Joback Method
hf	94.23	kJ/mol	Joback Method
hfus	14.59	kJ/mol	Joback Method
hvap	40.17	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.110		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	458.92	K	Joback Method
tc	678.24	K	Joback Method
tf	249.70 ± 0.30	K	NIST Webbook
tf	249.65 ± 0.30	K	NIST Webbook
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	240.06	J/mol×K	458.92	Joback Method
cpg	255.09	J/mol×K	495.47	Joback Method
cpg	269.14	J/mol×K	532.03	Joback Method
cpg	282.26	J/mol×K	568.58	Joback Method
cpg	294.51	J/mol×K	605.14	Joback Method
cpg	305.95	J/mol×K	641.69	Joback Method
cpg	316.62	J/mol×K	678.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.20	K	4.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C768003&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
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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