Benzene, (2-methyl-1-propenyl)-

Other names:	(2-METHYL-1-PROPENYL)BENZENE (2-Methylpropenyl)benzene 1,1-DIMETHYL-2-PHENYLETHYLENE 1-Phenyl-2-methyl-1-propene 1-Phenyl-2-methylpropene 1-Propene, 2-methyl-1-phenyl- 2-Methyl-1-phenyl-1-propene 2-Methyl-1-phenylpropene 2-methyl-1-propenylbenzene BETA,BETA-DIMETHYLSTYRENE Benzene, (2-methyl-1-propen-1-yl)- Benzene, (2-methylpropenyl)- Isobutenylbenzene NSC 163349 Propene, 2-methyl-1-phenyl- «beta»,«beta»-Dimethylstyrene «beta»-Methylisoallylbenzene Â«betaÂ»,Â«betaÂ»-Dimethylstyrene Â«betaÂ»-Methylisoallylbenzene
Inchi:	InChI=1S/C10H12/c1-9(2)8-10-6-4-3-5-7-10/h3-8H,1-2H3
InchiKey:	BTOVVHWKPVSLBI-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	CC(C)=Cc1ccccc1
Mol. weight [g/mol]:	132.20
CAS:	768-49-0

Physical Properties

Property code	Value	Unit	Source
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
ie	7.78 ± 0.04	eV	NIST Webbook
log10ws	-3.13		Crippen Method
logp	3.110		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method

rinpol	1071.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	177.60		NIST Webbook
rinpol	1067.00		NIST Webbook
tb	461.06 ± 0.25	K	NIST Webbook
tb	461.06 ± 0.30	K	NIST Webbook
tb	460.85 ± 0.40	K	NIST Webbook
tb	461.07 ± 0.30	K	NIST Webbook
tb	461.65 ± 2.00	K	NIST Webbook
tb	454.15 ± 4.00	K	NIST Webbook
tb	461.05 ± 0.30	K	NIST Webbook
tb	455.15 ± 5.00	K	NIST Webbook
tb	455.00 ± 4.00	K	NIST Webbook
tb	460.95 ± 1.50	K	NIST Webbook
tb	455.15 ± 3.00	K	NIST Webbook
tb	461.07 ± 0.40	K	NIST Webbook
tb	460.70	K	NIST Webbook
tb	454.15 ± 5.00	K	NIST Webbook
tc	678.24	K	Joback Method
tf	217.15 ± 3.00	K	NIST Webbook
tf	224.15 ± 2.00	K	NIST Webbook
tf	211.65 ± 5.00	K	NIST Webbook
tf	223.35 ± 1.50	K	NIST Webbook
tf	222.05 ± 0.20	K	NIST Webbook
tf	221.97 ± 0.20	K	NIST Webbook
tf	221.97 ± 0.30	K	NIST Webbook
tf	221.97 ± 0.20	K	NIST Webbook
tf	222.55 ± 0.20	K	NIST Webbook
tf	221.97 ± 0.30	K	NIST Webbook
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol730.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C768490&Units=SI

Legend

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume