Benzene, (2,2-dimethyl-1-methylenepropyl)-

Other names:	Styrene, «alpha»-tert-butyl-
	«alpha»-tert-Butylstyrene
	1-tert-Butyl-1-phenylethylene
	3,3-Dimethyl-2-phenylbutene
Inchi:	InChI=1S/C12H16/c1-10(12(2,3)4)11-8-6-5-7-9-11/h5-9H,1H2,2-4H3
InchiKey:	OJHQXSRIBZMCSR-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	C=C(c1ccccc1)C(C)(C)C
Mol. weight [g/mol]:	160.26
CAS:	5676-29-9

Physical Properties

Property code	Value	Unit	Source
affp	859.20	kJ/mol	NIST Webbook
basg	830.30	kJ/mol	NIST Webbook
gf	244.70	kJ/mol	Joback Method
hf	52.41	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	53.20 ± 0.10	kJ/mol	NIST Webbook
ie	8.25 ± 0.04	eV	NIST Webbook
log10ws	-3.73		Crippen Method
logp	3.746		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	493.97	K	Joback Method
tc	715.24	K	Joback Method
tf	238.12	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.94	J/mol×K	493.97	Joback Method
cpg	347.93	J/mol×K	530.85	Joback Method

cpg	364.66	J/mol×K	567.73	Joback Method
cpg	380.21	J/mol×K	604.60	Joback Method
cpg	394.66	J/mol×K	641.48	Joback Method
cpg	408.07	J/mol×K	678.36	Joback Method
cpg	420.52	J/mol×K	715.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5676299&Units=SI

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

affp: Proton affinity

basg: Gas basicity

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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume