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

Other names:	«alpha»,«beta»,«beta»-Trimethylstyrene
	2-Butene, 2-methyl-3-phenyl-
	2-Phenyl-3-methyl-2-butene
	Trimethylstyrene
Inchi:	InChI=1S/C11H14/c1-9(2)10(3)11-7-5-4-6-8-11/h4-8H,1-3H3
InchiKey:	ZTHJQCDAHYOPIK-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	CC(C)=C(C)c1ccccc1
Mol. weight [g/mol]:	146.23
CAS:	769-57-3

Physical Properties

Property code	Value	Unit	Source
chl	-6329.10	kJ/mol	NIST Webbook
gf	217.27	kJ/mol	Joback Method
hf	63.80	kJ/mol	Joback Method
hfus	15.87	kJ/mol	Joback Method
hvap	42.47	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.500		Crippen Method
mcvol	137.790	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	462.00 ± 3.00	K	NIST Webbook
tc	702.03	K	Joback Method
tf	207.15	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.03	J/mol×K	481.68	Joback Method
cpg	299.29	J/mol×K	518.41	Joback Method
cpg	314.50	J/mol×K	555.13	Joback Method
cpg	328.72	J/mol×K	591.86	Joback Method

cpg	342.00	J/mol×K	628.58	Joback Method
cpg	354.42	J/mol×K	665.31	Joback Method
cpg	366.01	J/mol×K	702.03	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C769573&Units=SI

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