

Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)-

Other names:	Styrene, o-isopropyl-«alpha»-methyl-
Inchi:	InChI=1S/C12H16/c1-9(2)11-7-5-6-8-12(11)10(3)4/h5-8,10H,1H2,2-4H3
InchiKey:	NQNOSJUXYMZTTF-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	<chem>C=C(C)c1cccc1C(C)C</chem>
Mol. weight [g/mol]:	160.26
CAS:	5557-93-7

Physical Properties

Property code	Value	Unit	Source
gf	229.79	kJ/mol	Joback Method
hf	44.41	kJ/mol	Joback Method
hfus	14.37	kJ/mol	Joback Method
hvap	44.27	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.843		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	501.74	K	Joback Method
tc	715.12	K	Joback Method
tf	233.22	K	Joback Method
vc	0.576	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.95	J/mol×K	501.74	Joback Method
cpg	344.58	J/mol×K	537.30	Joback Method
cpg	360.26	J/mol×K	572.87	Joback Method
cpg	375.02	J/mol×K	608.43	Joback Method
cpg	388.90	J/mol×K	644.00	Joback Method
cpg	401.95	J/mol×K	679.56	Joback Method
cpg	414.20	J/mol×K	715.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5557937&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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