# Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-

**Other names:** Styrene, m-isopropyl-«alpha»-methyl-
m-Isopropyl-«alpha»-methylstyrene
1-Isopropenyl-3-isopropylbenzene

**Inchi:** InChI=1S/C12H16/c1-9(2)11-6-5-7-12(8-11)10(3)4/h5-8,10H,1H2,2-4H3

**InchiKey:** BDXXZCIRCYKRBT-UHFFFAOYSA-N

**Formula:** C12H16

**SMILES:** C=C(C)c1cccc(C(C)C)c1

**Mol. weight [g/mol]:** 160.26

**CAS:** 1129-29-9

## 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 |
| rinpol | 1144.00 | | NIST Webbook |
| ripol | 1360.00 | | NIST Webbook |
| tb | 501.74 | K | Joback Method |
| tc | 715.12 | K | Joback Method |
| tf | 233.22 | K | Joback Method |
| vc | 0.576 | m3/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 |

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|---|---|---|---|---|
| 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

| | |
|---|---|
| **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=C1129299&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |