

Benzene, 1-ethenyl-4-(2-methylpropyl)-

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|-----------------------------|---|
| Other names: | 1-Isobutyl-4-vinylbenzene |
| Inchi: | InChI=1S/C12H16/c1-4-11-5-7-12(8-6-11)9-10(2)3/h4-8,10H,1,9H2,2-3H3 |
| InchiKey: | VTMSSJKVUVVWNJ-UHFFFAOYSA-N |
| Formula: | C12H16 |
| SMILES: | <chem>C=Cc1ccc(CC(C)C)cc1</chem> |
| Mol. weight [g/mol]: | 160.26 |
| CAS: | 63444-56-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 238.34 | kJ/mol | Joback Method |
| hf | 54.20 | kJ/mol | Joback Method |
| hfus | 15.68 | kJ/mol | Joback Method |
| hvap | 44.19 | kJ/mol | Joback Method |
| log10ws | -3.69 | | Crippen Method |
| logp | 3.528 | | Crippen Method |
| mcvol | 151.880 | ml/mol | McGowan Method |
| pc | 2490.03 | kPa | Joback Method |
| rinpol | 1228.00 | | NIST Webbook |
| tb | 501.86 | K | Joback Method |
| tc | 711.20 | K | Joback Method |
| tf | 247.18 | K | Joback Method |
| vc | 0.575 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 328.09 | J/molxK | 501.86 | Joback Method |
| cpg | 401.03 | J/molxK | 676.31 | Joback Method |
| cpg | 388.14 | J/molxK | 641.42 | Joback Method |
| cpg | 374.43 | J/molxK | 606.53 | Joback Method |
| cpg | 359.89 | J/molxK | 571.64 | Joback Method |
| cpg | 344.45 | J/molxK | 536.75 | Joback Method |
| cpg | 413.15 | J/molxK | 711.20 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001916 | Paxs | 501.86 | Joback Method |
| dvisc | 0.0002477 | Paxs | 459.41 | Joback Method |
| dvisc | 0.0003374 | Paxs | 416.97 | Joback Method |
| dvisc | 0.0004930 | Paxs | 374.52 | Joback Method |
| dvisc | 0.0007937 | Paxs | 332.07 | Joback Method |
| dvisc | 0.0014692 | Paxs | 289.63 | Joback Method |
| dvisc | 0.0033600 | Paxs | 247.18 | 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=C63444564&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| 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 |
| mvol: | 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 |

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