

Benzene, (1-chloro-1,2-dimethylpropyl)

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| Inchi: | InChI=1S/C11H15Cl/c1-9(2)11(3,12)10-7-5-4-6-8-10/h4-9H,1-3H3 |
| InchiKey: | HFXFGGPUUWNIU-UHFFFAOYSA-N |
| Formula: | C11H15Cl |
| SMILES: | CC(C)C(C)(Cl)c1ccccc1 |
| Mol. weight [g/mol]: | 182.69 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 142.62 | kJ/mol | Joback Method |
| hf | -63.61 | kJ/mol | Joback Method |
| hfus | 11.55 | kJ/mol | Joback Method |
| hvap | 45.06 | kJ/mol | Joback Method |
| log10ws | -3.61 | | Crippen Method |
| logp | 3.797 | | Crippen Method |
| mvol | 154.330 | ml/mol | McGowan Method |
| pc | 2621.78 | kPa | Joback Method |
| rinpol | 1262.00 | | NIST Webbook |
| rinpol | 1262.00 | | NIST Webbook |
| tb | 511.52 | K | Joback Method |
| tc | 737.70 | K | Joback Method |
| tf | 257.49 | K | Joback Method |
| vc | 0.576 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 333.28 | J/molxK | 511.52 | Joback Method |
| cpg | 406.44 | J/molxK | 700.01 | Joback Method |
| cpg | 393.96 | J/molxK | 662.31 | Joback Method |
| cpg | 380.47 | J/molxK | 624.61 | Joback Method |
| cpg | 365.91 | J/molxK | 586.91 | Joback Method |
| cpg | 350.21 | J/molxK | 549.22 | Joback Method |
| cpg | 417.99 | J/molxK | 737.70 | Joback Method |
| dvisc | 0.0002049 | Paxs | 511.52 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002829 | Paxs | 469.18 | Joback Method |
| dvisc | 0.0004165 | Paxs | 426.84 | Joback Method |
| dvisc | 0.0006677 | Paxs | 384.50 | Joback Method |
| dvisc | 0.0012030 | Paxs | 342.17 | Joback Method |
| dvisc | 0.0025593 | Paxs | 299.83 | Joback Method |
| dvisc | 0.0069791 | Paxs | 257.49 | 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=R131749&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.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 |
| mcvol: | 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 |

Latest version available from:

<https://www.chemeo.com/cid/31-477-8/Benzene-1-chloro-1-2-dimethylpropyl.pdf>

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