

Benzene, m-bis(1-methylbutyl)

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|-----------------------------|--|
| Inchi: | InChI=1S/C16H26/c1-5-8-13(3)15-10-7-11-16(12-15)14(4)9-6-2/h7,10-14H,5-6,8-9H2,1-4 |
| InchiKey: | UCASMHVYEXFFDH-UHFFFAOYSA-N |
| Formula: | C16H26 |
| SMILES: | CCCC(C)c1cccc(C(C)CCC)c1 |
| Mol. weight [g/mol]: | 218.38 |
| CAS: | 1020-38-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 181.74 | kJ/mol | Joback Method |
| hf | -159.07 | kJ/mol | Joback Method |
| hfus | 23.80 | kJ/mol | Joback Method |
| hvap | 53.37 | kJ/mol | Joback Method |
| log10ws | -5.52 | | Crippen Method |
| logp | 5.494 | | Crippen Method |
| mcvol | 212.540 | ml/mol | McGowan Method |
| pc | 1704.71 | kPa | Joback Method |
| tb | 596.26 | K | Joback Method |
| tc | 793.83 | K | Joback Method |
| tf | 279.02 | K | Joback Method |
| vc | 0.811 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 545.90 | J/molxK | 596.26 | Joback Method |
| cpg | 634.22 | J/molxK | 760.90 | Joback Method |
| cpg | 618.49 | J/molxK | 727.97 | Joback Method |
| cpg | 601.82 | J/molxK | 695.05 | Joback Method |
| cpg | 584.20 | J/molxK | 662.12 | Joback Method |
| cpg | 565.57 | J/molxK | 629.19 | Joback Method |
| cpg | 649.07 | J/molxK | 793.83 | Joback Method |
| dvisc | 0.0001293 | Paxs | 596.26 | Joback Method |
| dvisc | 0.0001756 | Paxs | 543.39 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002546 | Paxs | 490.51 | Joback Method |
| dvisc | 0.0004041 | Paxs | 437.64 | Joback Method |
| dvisc | 0.0007280 | Paxs | 384.77 | Joback Method |
| dvisc | 0.0015822 | Paxs | 331.89 | Joback Method |
| dvisc | 0.0046147 | Paxs | 279.02 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1020388&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 |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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