

1,2,4-Tri-isopropylbenzene

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|-----------------------------|--|
| Other names: | Benzene, 1,2,4-tris(1-methylethyl)- |
| Inchi: | InChI=1S/C15H24/c1-10(2)13-7-8-14(11(3)4)15(9-13)12(5)6/h7-12H,1-6H3 |
| InchiKey: | RWGMANKDYBWN NP-UHFFFAOYSA-N |
| Formula: | C15H24 |
| SMILES: | CC(C)c1ccc(C(C)C)c(C(C)C)c1 |
| Mol. weight [g/mol]: | 204.35 |
| CAS: | 948-32-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|----------------------|----------------|
| gf | 161.25 | kJ/mol | Joback Method |
| hf | -155.18 | kJ/mol | Joback Method |
| hfus | 17.30 | kJ/mol | Joback Method |
| hvap | 51.42 | kJ/mol | Joback Method |
| log10ws | -5.03 | | Crippen Method |
| logp | 5.057 | | Crippen Method |
| mcvol | 198.450 | ml/mol | McGowan Method |
| pc | 1837.26 | kPa | Joback Method |
| rinpol | 1201.00 | | NIST Webbook |
| ripol | 1524.00 | | NIST Webbook |
| ripol | 1528.00 | | NIST Webbook |
| ripol | 1532.00 | | NIST Webbook |
| ripol | 1540.00 | | NIST Webbook |
| ripol | 1520.00 | | NIST Webbook |
| tb | 517.20 | K | NIST Webbook |
| tb | 512.00 ± 2.00 | K | NIST Webbook |
| tc | 783.37 | K | Joback Method |
| tf | 265.27 | K | Joback Method |
| vc | 0.750 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 494.44 | J/mol×K | 577.92 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 581.61 | J/molxK | 749.13 | Joback Method |
| cpg | 566.10 | J/molxK | 714.89 | Joback Method |
| cpg | 549.66 | J/molxK | 680.65 | Joback Method |
| cpg | 532.26 | J/molxK | 646.40 | Joback Method |
| cpg | 513.86 | J/molxK | 612.16 | Joback Method |
| cpg | 596.23 | J/molxK | 783.37 | Joback Method |
| dvisc | 0.0001301 | Paxs | 577.92 | Joback Method |
| dvisc | 0.0001761 | Paxs | 525.81 | Joback Method |
| dvisc | 0.0002549 | Paxs | 473.70 | Joback Method |
| dvisc | 0.0004043 | Paxs | 421.59 | Joback Method |
| dvisc | 0.0007301 | Paxs | 369.49 | Joback Method |
| dvisc | 0.0016012 | Paxs | 317.38 | Joback Method |
| dvisc | 0.0047804 | Paxs | 265.27 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 386.70 | K | 1.90 | NIST Webbook |

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=C948323&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

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|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcpvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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