

Benzene, 1,3,5-tris(1-methylpropyl)-

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|-----------------------------|-----------------------------------------------------------------------------------------|
| Other names: | Benzene, 1,3,5-tri-sec-butyl- 1,3,5-Tri-sec-butylbenzene 1,3,5-Tri-s-butylbenzene |
| Inchi: | InChI=1S/C18H30/c1-7-13(4)16-10-17(14(5)8-2)12-18(11-16)15(6)9-3/h10-15H,7-9H2,1- |
| InchiKey: | LNCLJYZMKXSECB-UHFFFAOYSA-N |
| Formula: | C18H30 |
| SMILES: | CCC(C)c1cc(C(C)CC)cc(C(C)CC)c1 |
| Mol. weight [g/mol]: | 246.43 |
| CAS: | 6565-55-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 186.51 | kJ/mol | Joback Method |
| hf | -217.10 | kJ/mol | Joback Method |
| hfus | 25.07 | kJ/mol | Joback Method |
| hvap | 58.10 | kJ/mol | Joback Method |
| log10ws | -6.28 | | Crippen Method |
| logp | 6.227 | | Crippen Method |
| mcvol | 240.720 | ml/mol | McGowan Method |
| pc | 1455.68 | kPa | Joback Method |
| tb | 646.56 | K | Joback Method |
| tc | 843.63 | K | Joback Method |
| tf | 299.08 | K | Joback Method |
| vc | 0.917 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 655.31 | J/molxK | 646.56 | Joback Method |
| cpg | 747.40 | J/molxK | 810.78 | Joback Method |
| cpg | 730.99 | J/molxK | 777.94 | Joback Method |
| cpg | 713.62 | J/molxK | 745.09 | Joback Method |
| cpg | 695.24 | J/molxK | 712.25 | Joback Method |
| cpg | 675.81 | J/molxK | 679.40 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 762.88 | J/mol×K | 843.63 | Joback Method |
| dvisc | 0.0000966 | Paxs | 646.56 | Joback Method |
| dvisc | 0.0001320 | Paxs | 588.65 | Joback Method |
| dvisc | 0.0001930 | Paxs | 530.73 | Joback Method |
| dvisc | 0.0003097 | Paxs | 472.82 | Joback Method |
| dvisc | 0.0005672 | Paxs | 414.91 | Joback Method |
| dvisc | 0.0012641 | Paxs | 356.99 | Joback Method |
| dvisc | 0.0038426 | Paxs | 299.08 | 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=C6565555&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|-------------------------------------------------|
| 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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<https://www.chemeo.com/cid/23-805-2/Benzene-1-3-5-tris-1-methylpropyl.pdf>

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