

Benzene, 1,4-diethyl-2-methyl-

| | |
|-----------------------------|---|
| Other names: | 1,4-Diethyl-2-methylbenzene 1-Methyl-2,5-diethylbenzene Benzene, 2,5-diethyl-1-methyl |
| Inchi: | InChI=1S/C11H16/c1-4-10-6-7-11(5-2)9(3)8-10/h6-8H,4-5H2,1-3H3 |
| InchiKey: | ZEHGGUIGEDITMM-UHFFFAOYSA-N |
| Formula: | C11H16 |
| SMILES: | CCc1ccc(CC)c(C)c1 |
| Mol. weight [g/mol]: | 148.24 |
| CAS: | 13632-94-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | 134.89 | kJ/mol | Joback Method |
| hf | -56.78 | kJ/mol | Joback Method |
| hfus | 17.51 | kJ/mol | Joback Method |
| hvap | 43.68 | kJ/mol | Joback Method |
| log10ws | -3.55 | | Crippen Method |
| logp | 3.120 | | Crippen Method |
| mcvol | 142.090 | ml/mol | McGowan Method |
| pc | 2568.89 | kPa | Joback Method |
| rinpol | 1144.00 | | NIST Webbook |
| rinpol | 1164.00 | | NIST Webbook |
| rinpol | 1155.00 | | NIST Webbook |
| rinpol | 1144.00 | | NIST Webbook |
| rinpol | 1144.20 | | NIST Webbook |
| rinpol | 1143.30 | | NIST Webbook |
| rinpol | 1143.70 | | NIST Webbook |
| rinpol | 1144.00 | | NIST Webbook |
| rinpol | 1143.00 | | NIST Webbook |
| rinpol | 1149.00 | | NIST Webbook |
| ripol | 1404.00 | | NIST Webbook |
| ripol | 1415.00 | | NIST Webbook |
| ripol | 1427.00 | | NIST Webbook |
| ripol | 1403.60 | | NIST Webbook |
| ripol | 1425.00 | | NIST Webbook |
| ripol | 1404.00 | | NIST Webbook |
| ripol | 1415.00 | | NIST Webbook |

| | | | |
|-------|---------------|----------------------|---------------|
| ripol | 1464.00 | | NIST Webbook |
| ripol | 1453.00 | | NIST Webbook |
| ripol | 1440.00 | | NIST Webbook |
| ripol | 1425.00 | | NIST Webbook |
| tb | 479.00 ± 6.00 | K | NIST Webbook |
| tc | 692.15 | K | Joback Method |
| tf | 265.19 | K | Joback Method |
| vc | 0.543 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 301.47 | J/mol×K | 487.72 | Joback Method |
| cpg | 316.73 | J/mol×K | 521.79 | Joback Method |
| cpg | 331.23 | J/mol×K | 555.86 | Joback Method |
| cpg | 345.01 | J/mol×K | 589.93 | Joback Method |
| cpg | 358.09 | J/mol×K | 624.00 | Joback Method |
| cpg | 370.48 | J/mol×K | 658.08 | Joback Method |
| cpg | 382.22 | J/mol×K | 692.15 | Joback Method |
| dvisc | 0.0018138 | Paxs | 265.19 | Joback Method |
| dvisc | 0.0010046 | Paxs | 302.28 | Joback Method |
| dvisc | 0.0006331 | Paxs | 339.37 | Joback Method |
| dvisc | 0.0004370 | Paxs | 376.46 | Joback Method |
| dvisc | 0.0003223 | Paxs | 413.54 | Joback Method |
| dvisc | 0.0002500 | Paxs | 450.63 | Joback Method |
| dvisc | 0.0002015 | Paxs | 487.72 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.43838e+01 |
| Coeff. B | -3.97213e+03 |
| Coeff. C | -7.34990e+01 |
| Temperature range (K), min. | 355.29 |
| Temperature range (K), max. | 511.33 |

Sources

| | |
|---|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| 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=C13632945&Units=SI |
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |
| pvap: | Vapor pressure |
| rinpol: | Non-polar retention indices |
| ripol: | 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/72-377-4/Benzene-1-4-diethyl-2-methyl.pdf>

Generated by Cheméo on 2024-04-20 02:51:31.424926968 +0000 UTC m=+15870740.345504281.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.