

Benzene, (1-methylpropoxy)-

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|-----------------------------|--|
| Other names: | Ether, sec-butyl phenyl sec-Butoxybenzene sec-Butyl phenyl ether 2-Butyl phenyl ether |
| Inchi: | InChI=1S/C10H14O/c1-3-9(2)11-10-7-5-4-6-8-10/h4-9H,3H2,1-2H3 |
| InchiKey: | VJQIPKNMASGCOC-UHFFFAOYSA-N |
| Formula: | C10H14O |
| SMILES: | CCC(C)Oc1ccccc1 |
| Mol. weight [g/mol]: | 150.22 |
| CAS: | 10574-17-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|----------------------|----------------|
| gf | 38.29 | kJ/mol | Joback Method |
| hf | -150.70 | kJ/mol | Joback Method |
| hfus | 13.36 | kJ/mol | Joback Method |
| hvap | 42.15 | kJ/mol | Joback Method |
| log10ws | -2.96 | | Crippen Method |
| logp | 2.864 | | Crippen Method |
| mcvol | 133.870 | ml/mol | McGowan Method |
| pc | 2902.98 | kPa | Joback Method |
| tb | 466.15 ± 3.00 | K | NIST Webbook |
| tb | 467.70 | K | NIST Webbook |
| tc | 684.68 | K | Joback Method |
| tf | 236.11 | K | Joback Method |
| vc | 0.499 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 281.20 | J/mol×K | 476.86 | Joback Method |
| cpg | 296.31 | J/mol×K | 511.50 | Joback Method |
| cpg | 310.65 | J/mol×K | 546.13 | Joback Method |
| cpg | 324.23 | J/mol×K | 580.77 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 337.07 | J/molxK | 615.41 | Joback Method |
| cpg | 349.19 | J/molxK | 650.05 | Joback Method |
| cpg | 360.62 | J/molxK | 684.68 | Joback Method |
| dvisc | 0.0040774 | Paxs | 236.11 | Joback Method |
| dvisc | 0.0016757 | Paxs | 276.24 | Joback Method |
| dvisc | 0.0008630 | Paxs | 316.36 | Joback Method |
| dvisc | 0.0005160 | Paxs | 356.49 | Joback Method |
| dvisc | 0.0003424 | Paxs | 396.61 | Joback Method |
| dvisc | 0.0002450 | Paxs | 436.74 | Joback Method |
| dvisc | 0.0001854 | Paxs | 476.86 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 344.20 | K | 0.70 | NIST Webbook |

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=C10574171&Units=SI |
| 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 |
| 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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