

Octane, 1,1'-oxybis-

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| Other names: | 1,1'-Oxybisoctane 1-(Octyloxy)octane Antar Caprylic ether Di-n-octyl ether Dicaprylyl ether Dioctyl ether Ether, di-n-octyl- NSC 28948 Octyl ether bis(1-octyl) ether cetiol OE n-Octyl ether |
| Inchi: | InChI=1S/C16H34O/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h3-16H2,1-2H3 |
| InchiKey: | NKJOXAZJBOMXID-UHFFFAOYSA-N |
| Formula: | C16H34O |
| SMILES: | CCCCCCCCOCCCCCCCC |
| Mol. weight [g/mol]: | 242.44 |
| CAS: | 629-82-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | -21.16 | kJ/mol | Joback Method |
| hf | -505.79 | kJ/mol | Joback Method |
| hfus | 38.38 | kJ/mol | Joback Method |
| hvap | 53.62 | kJ/mol | Joback Method |
| log10ws | -5.61 | | Crippen Method |
| logp | 5.724 | | Crippen Method |
| mcvol | 242.170 | ml/mol | McGowan Method |
| pc | 1302.35 | kPa | Joback Method |
| rinpol | 1657.00 | | NIST Webbook |
| rinpol | 1657.00 | | NIST Webbook |
| rinpol | 1660.00 | | NIST Webbook |
| ripol | 1761.00 | | NIST Webbook |
| ripol | 1760.00 | | NIST Webbook |
| ripol | 1763.00 | | NIST Webbook |
| ripol | 1763.00 | | NIST Webbook |

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| ripol | 1761.00 | | NIST Webbook |
| tb | 559.70 ± 1.50 | K | NIST Webbook |
| tb | 559.70 | K | NIST Webbook |
| tc | 723.00 | K | Critical properties of some aliphatic symmetrical ethers |
| tf | 265.60 ± 1.00 | K | NIST Webbook |
| vc | 0.950 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 643.59 | J/mol×K | 587.90 | Joback Method |
| cpg | 662.46 | J/mol×K | 614.43 | Joback Method |
| cpg | 680.61 | J/mol×K | 640.97 | Joback Method |
| cpg | 698.07 | J/mol×K | 667.50 | Joback Method |
| cpg | 714.84 | J/mol×K | 694.03 | Joback Method |
| cpg | 730.94 | J/mol×K | 720.56 | Joback Method |
| cpg | 746.38 | J/mol×K | 747.10 | Joback Method |
| dvisc | 0.0033879 | Paxs | 292.31 | Joback Method |
| dvisc | 0.0013014 | Paxs | 341.57 | Joback Method |
| dvisc | 0.0006363 | Paxs | 390.84 | Joback Method |
| dvisc | 0.0003651 | Paxs | 440.11 | Joback Method |
| dvisc | 0.0002343 | Paxs | 489.37 | Joback Method |
| dvisc | 0.0001631 | Paxs | 538.63 | Joback Method |
| dvisc | 0.0001206 | Paxs | 587.90 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.55254e+01 |
| Coeff. B | -5.04961e+03 |
| Coeff. C | -9.67330e+01 |
| Temperature range (K), min. | 428.12 |
| Temperature range (K), max. | 591.12 |

| Information | Value |
|-----------------------------|--|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A | 1.98579e+02 |
| Coeff. B | -1.79056e+04 |
| Coeff. C | -2.61592e+01 |
| Coeff. D | 1.13104e-05 |
| Temperature range (K), min. | 265.55 |
| Temperature range (K), max. | 707.00 |

Sources

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|--|---|
| Critical properties of some aliphatic symmetrical ethers: KDB Vapor Pressure Data: | https://www.doi.org/10.1016/j.jct.2013.09.019 |
| Crippen Method: | https://www.chemec.org/research/kdb/hcprop/showprop.php?cmpid=1026 |
| Joback Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| KDB: | https://en.wikipedia.org/wiki/Joback_method |
| The Yaws Handbook of Vapor Pressure: NIST Webbook: | https://www.thermo.com/files/research/kdb/mol/mol1027.mol |
| Crippen Method: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| Chemical Equilibrium of the Liquid-Phase Dehydration of 1-Octanol to Cyclohexanone: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C629823&Units=SI |
| McGowan Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| | https://www.doi.org/10.1021/je301236k |
| | http://link.springer.com/article/10.1007/BF02311772 |

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 |
| mccol: | 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

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