

Butyl docosyl ether

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|-----------------------------|--|
| Inchi: | InChI=1S/C26H54O/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26-27 |
| InchiKey: | BATGFXRKHSIQIS-UHFFFAOYSA-N |
| Formula: | C26H54O |
| SMILES: | CCCCCCCCCCCCCCCCCCCCOCCCC |
| Mol. weight [g/mol]: | 382.71 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 63.04 | kJ/mol | Joback Method |
| hf | -712.19 | kJ/mol | Joback Method |
| hfus | 64.28 | kJ/mol | Joback Method |
| hvap | 75.88 | kJ/mol | Joback Method |
| log10ws | -9.79 | | Crippen Method |
| logp | 9.625 | | Crippen Method |
| mcvol | 383.070 | ml/mol | McGowan Method |
| pc | 718.37 | kPa | Joback Method |
| rinpol | 2673.00 | | NIST Webbook |
| tb | 816.70 | K | Joback Method |
| tc | 1000.19 | K | Joback Method |
| tf | 405.01 | K | Joback Method |
| vc | 1.510 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1252.62 | J/molxK | 816.70 | Joback Method |
| cpg | 1276.69 | J/molxK | 847.28 | Joback Method |
| cpg | 1299.51 | J/molxK | 877.86 | Joback Method |
| cpg | 1321.15 | J/molxK | 908.44 | Joback Method |
| cpg | 1341.63 | J/molxK | 939.02 | Joback Method |
| cpg | 1361.00 | J/molxK | 969.61 | Joback Method |
| cpg | 1379.30 | J/molxK | 1000.19 | Joback Method |
| dvisc | 0.0011802 | Paxs | 405.01 | Joback Method |
| dvisc | 0.0004212 | Paxs | 473.62 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0001951 | Paxs | 542.24 | Joback Method |
| dvisc | 0.0001074 | Paxs | 610.86 | Joback Method |
| dvisc | 0.0000667 | Paxs | 679.47 | Joback Method |
| dvisc | 0.0000452 | Paxs | 748.09 | Joback Method |
| dvisc | 0.0000327 | Paxs | 816.70 | 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=U406408&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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