

Octacosane, 9-methyl

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C29H60/c1-4-6-8-10-12-13-14-15-16-17-18-19-20-21-22-24-26-28-29(3)27-25 |
| InchiKey: | HGHNLISXMMUYAJ-UHFFFAOYSA-N |
| Formula: | C29H60 |
| SMILES: | CCCCCCCCCCCCCCCCCCCC(C)CCCCCCCC |
| Mol. weight [g/mol]: | 408.79 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 190.86 | kJ/mol | Joback Method |
| hf | -647.17 | kJ/mol | Joback Method |
| hfus | 67.34 | kJ/mol | Joback Method |
| hvap | 79.76 | kJ/mol | Joback Method |
| log10ws | -11.72 | | Crippen Method |
| logp | 11.415 | | Crippen Method |
| mcvol | 419.470 | ml/mol | McGowan Method |
| pc | 626.88 | kPa | Joback Method |
| rinsol | 2839.10 | | NIST Webbook |
| tb | 862.48 | K | Joback Method |
| tc | 1058.99 | K | Joback Method |
| tf | 401.59 | K | Joback Method |
| vc | 1.653 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1415.09 | J/molxK | 862.48 | Joback Method |
| cpg | 1532.71 | J/molxK | 1026.24 | Joback Method |
| cpg | 1511.74 | J/molxK | 993.49 | Joback Method |
| cpg | 1489.57 | J/molxK | 960.74 | Joback Method |
| cpg | 1466.11 | J/molxK | 927.98 | Joback Method |
| cpg | 1441.31 | J/molxK | 895.23 | Joback Method |
| cpg | 1552.54 | J/molxK | 1058.99 | Joback Method |
| dvisc | 0.0000258 | Paxs | 862.48 | Joback Method |
| dvisc | 0.0000366 | Paxs | 785.66 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000560 | Paxs | 708.85 | Joback Method |
| dvisc | 0.0000949 | Paxs | 632.04 | Joback Method |
| dvisc | 0.0001863 | Paxs | 555.22 | Joback Method |
| dvisc | 0.0004537 | Paxs | 478.40 | Joback Method |
| dvisc | 0.0015539 | Paxs | 401.59 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=R570897&Units=SI |

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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<https://www.chemeo.com/cid/63-322-4/Octacosane-9-methyl.pdf>

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