# Octadecane, 1-iodo-

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|---|---|
| **Other names:** | 1-Iodooctadecane |
| | Octadecyl iodide |
| | Stearyl iodide |
| | n-Octadecyl iodide |
| **Inchi:** | InChI=1S/C18H37I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h2-18H2,1H3 |
| **InchiKey:** | ZNJOCVLVYVOUGB-UHFFFAOYSA-N |
| **Formula:** | C18H37I |
| **SMILES:** | CCCCCCCCCCCCCCCCCCI |
| **Mol. weight [g/mol]:** | 380.39 |
| **CAS:** | 629-93-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 158.80 | kJ/mol | Joback Method |
| hf | -337.98 | kJ/mol | Joback Method |
| hfus | 46.78 | kJ/mol | Joback Method |
| hvap | 109.30 | kJ/mol | NIST Webbook |
| log10ws | -8.31 | | Crippen Method |
| logp | 7.683 | | Crippen Method |
| mcvol | 290.300 | ml/mol | McGowan Method |
| pc | 1135.20 | kPa | Joback Method |
| rinpol | 2290.00 | | NIST Webbook |
| rinpol | 2290.00 | | NIST Webbook |
| rinpol | 2240.00 | | NIST Webbook |
| rinpol | 2272.00 | | NIST Webbook |
| ripol | 2576.00 | | NIST Webbook |
| tb | 656.20 | K | NIST Webbook |
| tc | 883.65 | K | Joback Method |
| tf | 307.00 ± 3.00 | K | NIST Webbook |
| vc | 1.131 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 803.35 | J/mol×K | 704.38 | Joback Method |
| cpg | 822.42 | J/mol×K | 734.26 | Joback Method |
| cpg | 840.60 | J/mol×K | 764.14 | Joback Method |
| cpg | 857.92 | J/mol×K | 794.02 | Joback Method |
| cpg | 874.42 | J/mol×K | 823.90 | Joback Method |
| cpg | 890.14 | J/mol×K | 853.77 | Joback Method |
| cpg | 905.12 | J/mol×K | 883.65 | Joback Method |
| dvisc | 0.0028659 | Pa×s | 350.68 | Joback Method |
| dvisc | 0.0010877 | Pa×s | 409.63 | Joback Method |
| dvisc | 0.0005268 | Pa×s | 468.58 | Joback Method |
| dvisc | 0.0003000 | Pa×s | 527.53 | Joback Method |
| dvisc | 0.0001913 | Pa×s | 586.48 | Joback Method |
| dvisc | 0.0001325 | Pa×s | 645.43 | Joback Method |
| dvisc | 0.0000975 | Pa×s | 704.38 | Joback Method |
| hvapt | 77.20 | kJ/mol | 584.50 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 468.70 | K | 0.30 | NIST Webbook |
| tbrp | 468.50 ± 1.50 | K | 0.30 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.63563e+01 |
| Coeff. B | -6.04763e+03 |
| Coeff. C | -1.23560e+02 |
| Temperature range (K), min. | 499.92 |
| Temperature range (K), max. | 671.11 |

# 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=C629936&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/ci990307l |

# 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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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