

Formic acid, octyl ester

Other names: FORMIC ACID,OCTYL ESTER

Octyl alcohol, formate

Octyl formate

Octyl formiate

Octyl methanoate

n-Octyl formate

n-Octyl methanoate

Inchi: InChI=1S/C9H18O2/c1-2-3-4-5-6-7-8-11-9-10/h9H,2-8H2,1H3

InchiKey: AVBRYQRTMPHARE-UHFFFAOYSA-N

Formula: C9H18O2

SMILES: CCCCCCCCOC=O

Mol. weight [g/mol]: 158.24

CAS: 112-32-3

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|--------|----------------|
| gf | -179.62 | kJ/mol | Joback Method |
| hf | -446.89 | kJ/mol | Joback Method |
| hfus | 22.54 | kJ/mol | Joback Method |
| hvap | 44.76 | kJ/mol | Joback Method |
| log10ws | -2.45 | | Crippen Method |
| logp | 2.520 | | Crippen Method |
| mcvol | 145.110 | ml/mol | McGowan Method |
| pc | 2438.65 | kPa | Joback Method |
| rinpol | 1112.00 | | NIST Webbook |
| rinpol | 1109.00 | | NIST Webbook |
| rinpol | 1117.00 | | NIST Webbook |
| rinpol | 1117.00 | | NIST Webbook |
| rinpol | 1128.00 | | NIST Webbook |
| rinpol | 1128.00 | | NIST Webbook |
| rinpol | 1110.00 | | NIST Webbook |
| rinpol | 1104.00 | | NIST Webbook |
| ripol | 1560.00 | | NIST Webbook |
| ripol | 1560.00 | | NIST Webbook |
| tb | 471.95 ± 0.30 | K | NIST Webbook |
| tb | 471.30 ± 1.50 | K | NIST Webbook |
| tb | 471.00 ± 3.00 | K | NIST Webbook |

| | | | |
|----|---------------|---------|---------------|
| tb | 471.95 | K | KDB |
| tc | 645.86 | K | Joback Method |
| tf | 234.10 ± 0.50 | K | NIST Webbook |
| tf | 234.05 | K | KDB |
| vc | 0.575 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------------------------------------------------------------|
| cpg | 394.42 | J/mol×K | 645.86 | Joback Method |
| cpg | 336.68 | J/mol×K | 504.64 | Joback Method |
| cpg | 349.13 | J/mol×K | 532.89 | Joback Method |
| cpg | 361.12 | J/mol×K | 561.13 | Joback Method |
| cpg | 372.67 | J/mol×K | 589.37 | Joback Method |
| cpg | 383.77 | J/mol×K | 617.62 | Joback Method |
| cpg | 323.77 | J/mol×K | 476.40 | Joback Method |
| dvisc | 0.0037595 | Paxs | 255.42 | Joback Method |
| dvisc | 0.0018180 | Paxs | 292.25 | Joback Method |
| dvisc | 0.0010344 | Paxs | 329.08 | Joback Method |
| dvisc | 0.0006593 | Paxs | 365.91 | Joback Method |
| dvisc | 0.0004563 | Paxs | 402.74 | Joback Method |
| dvisc | 0.0003359 | Paxs | 439.57 | Joback Method |
| dvisc | 0.0002592 | Paxs | 476.40 | Joback Method |
| pvap | 0.55 | kPa | 335.30 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.49 | kPa | 333.40 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.66 | kPa | 338.30 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.43 | kPa | 331.30 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.37 | kPa | 328.40 | Vapour pressures and enthalpies of vaporization of aliphatic esters |

| | | | | |
|------|------|-----|--------|---------------------------------------------------------------------|
| pvap | 0.27 | kPa | 323.50 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.19 | kPa | 318.50 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.14 | kPa | 313.50 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.09 | kPa | 308.20 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.06 | kPa | 303.20 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.06 | kPa | 303.20 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.04 | kPa | 298.40 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.03 | kPa | 293.30 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.02 | kPa | 290.80 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.02 | kPa | 288.20 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.02 | kPa | 285.70 | Vapour pressures and enthalpies of vaporization of aliphatic esters |
| pvap | 0.01 | kPa | 283.30 | Vapour pressures and enthalpies of vaporization of aliphatic esters |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.56616e+01 |
| Coeff. B | -4.40178e+03 |
| Coeff. C | -7.24080e+01 |
| Temperature range (K), min. | 358.72 |
| Temperature range (K), max. | 497.69 |

| Information | Value |
|-----------------------------|--------------------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$ |
| Coeff. A | 7.89702e+01 |
| Coeff. B | -8.58676e+03 |
| Coeff. C | -9.33680e+00 |
| Coeff. D | 5.95103e-06 |
| Temperature range (K), min. | 234.05 |
| Temperature range (K), max. | 645.00 |

Sources

| | |
|---------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| The Yaws Handbook of Vapor Pressure: KDB: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure https://www.cheric.org/files/research/kdb/mol/mol1117.mol |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C112323&Units=SI |
| Vapour pressures and enthalpies of vaporization of aliphatic esters: KDB Vapor Pressure Data: | https://www.doi.org/10.1016/j.fluid.2012.08.003 https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1117 |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| 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 |
| 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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