# Ethanol, 2-(octylthio)-

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|---|---|
| **Other names:** | MGK Repellent 874 |
| | MGK 874 |
| | R-874 |
| | 2-(Octylthio)ethanol |
| | 2-Hydroxyethyl n-octyl sulfide |
| | 2-Hydroxyethyl octyl sulfide |
| | «beta»-Hydroxyethyl n-octyl sulfide |
| | r-874 Phillips |
| | MGK repellent R-874 |
| | 2-(Oktylthio)ethanol |
| | NSC 163967 |
| **Inchi:** | InChI=1S/C10H22OS/c1-2-3-4-5-6-7-9-12-10-8-11/h11H,2-10H2,1H3 |
| **InchiKey:** | KXPXKNBDCUOENF-UHFFFAOYSA-N |
| **Formula:** | C10H22OS |
| **SMILES:** | CCCCCCCCSCCO |
| **Mol. weight [g/mol]:** | 190.35 |
| **CAS:** | 3547-33-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -70.38 | kJ/mol | Joback Method |
| hf | -360.09 | kJ/mol | Joback Method |
| hfus | 29.87 | kJ/mol | Joback Method |
| hvap | 61.35 | kJ/mol | Joback Method |
| log10ws | -3.16 | | Crippen Method |
| logp | 3.072 | | Crippen Method |
| mcvol | 173.980 | ml/mol | McGowan Method |
| pc | 2336.03 | kPa | Joback Method |
| rinpol | 1562.00 | | NIST Webbook |
| rinpol | 1562.00 | | NIST Webbook |
| tb | 589.16 | K | Joback Method |
| tc | 763.42 | K | Joback Method |
| tf | 297.68 | K | Joback Method |
| vc | 0.668 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 438.61 | J/mol×K | 589.16 | Joback Method |
| cpg | 452.10 | J/mol×K | 618.20 | Joback Method |
| cpg | 465.00 | J/mol×K | 647.25 | Joback Method |
| cpg | 477.35 | J/mol×K | 676.29 | Joback Method |
| cpg | 489.13 | J/mol×K | 705.34 | Joback Method |
| cpg | 500.38 | J/mol×K | 734.38 | Joback Method |
| cpg | 511.11 | J/mol×K | 763.42 | Joback Method |

# Sources

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|---|---|
| **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=C3547339&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |