# Thiophene, 2-ethyl-

**Other names:** 2-Ethylthiophene
2-Ethylthiophenol
**Inchi:** InChI=1S/C6H8S/c1-2-6-4-3-5-7-6/h3-5H,2H2,1H3
**InchiKey:** JCCCMAAJYSNBPR-UHFFFAOYSA-N
**Formula:** C6H8S
**SMILES:** CCc1cccs1
**Mol. weight [g/mol]:** 112.19
**CAS:** 872-55-9

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hvap | 39.70 ± 0.90 | kJ/mol | NIST Webbook |
| ie | 8.67 ± 0.05 | eV | NIST Webbook |
| ie | 8.80 ± 0.20 | eV | NIST Webbook |
| ie | 8.57 | eV | NIST Webbook |
| log10ws | -2.59 | | Aqueous Solubility Prediction Method |
| logp | 2.310 | | Crippen Method |
| mcvol | 92.290 | ml/mol | McGowan Method |
| rinpol | 872.00 | | NIST Webbook |
| rinpol | 850.00 | | NIST Webbook |
| rinpol | 850.00 | | NIST Webbook |
| rinpol | 845.00 | | NIST Webbook |
| rinpol | 905.00 | | NIST Webbook |
| rinpol | 871.00 | | NIST Webbook |
| rinpol | 846.00 | | NIST Webbook |
| rinpol | 847.00 | | NIST Webbook |
| rinpol | 871.00 | | NIST Webbook |
| rinpol | 880.00 | | NIST Webbook |
| rinpol | 870.00 | | NIST Webbook |
| rinpol | 870.00 | | NIST Webbook |
| rinpol | 872.00 | | NIST Webbook |
| rinpol | 905.00 | | NIST Webbook |
| rinpol | 868.00 | | NIST Webbook |
| rinpol | 871.00 | | NIST Webbook |
| rinpol | 861.00 | | NIST Webbook |
| rinpol | 844.00 | | NIST Webbook |

| | | | |
|---|---|---|---|
| rinpol | 844.00 | | NIST Webbook |
| rinpol | 869.00 | | NIST Webbook |
| rinpol | 874.00 | | NIST Webbook |
| rinpol | 837.00 | | NIST Webbook |
| rinpol | 850.00 | | NIST Webbook |
| rinpol | 847.00 | | NIST Webbook |
| rinpol | 874.00 | | NIST Webbook |
| rinpol | 845.00 | | NIST Webbook |
| rinpol | 846.00 | | NIST Webbook |
| rinpol | 845.00 | | NIST Webbook |
| rinpol | 846.00 | | NIST Webbook |
| rinpol | 868.00 | | NIST Webbook |
| rinpol | 871.00 | | NIST Webbook |
| rinpol | 861.00 | | NIST Webbook |
| rinpol | 851.00 | | NIST Webbook |
| rinpol | 845.00 | | NIST Webbook |
| ripol | 1179.00 | | NIST Webbook |
| ripol | 1177.00 | | NIST Webbook |
| ripol | 1167.00 | | NIST Webbook |
| ripol | 1161.00 | | NIST Webbook |
| ripol | 1162.00 | | NIST Webbook |
| ripol | 1179.00 | | NIST Webbook |
| ripol | 1170.00 | | NIST Webbook |
| ripol | 1170.00 | | NIST Webbook |
| ripol | 1191.00 | | NIST Webbook |
| ripol | 1185.00 | | NIST Webbook |
| ripol | 1183.00 | | NIST Webbook |
| ripol | 1162.00 | | NIST Webbook |
| ripol | 1173.00 | | NIST Webbook |
| ripol | 1180.00 | | NIST Webbook |
| ripol | 1182.00 | | NIST Webbook |
| ripol | 1172.00 | | NIST Webbook |
| ripol | 1182.00 | | NIST Webbook |
| ripol | 1177.00 | | NIST Webbook |
| ripol | 1180.00 | | NIST Webbook |
| tb | 407.15 | K | Isobaric vapor-liquid equilibrium for binary systemof 2-ethylthiophene + n-octane at 101.33 kPa |
| tb | 407.14 | K | Phase equilibria of three binary systems containing 2,5-dimethylthiophene and 2-ethylthiophene in hydrocarbons |
| tb | 407.20 | K | NIST Webbook |
| tb | 406.15 ± 2.00 | K | NIST Webbook |
| tb | 407.00 ± 4.00 | K | NIST Webbook |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| hvapt | 39.70 | kJ/mol | 353.50 | NIST Webbook |
| pvap | 101.33 | kPa | 407.15 | Isobaric vapor-liquid equilibrium for binary systemof 2-ethylthiophene + n-octane at 101.33 kPa |
| pvap | 101.33 | kPa | 407.14 | Phase equilibria of three binary systems containing 2,5-dimethylthiophene and 2-ethylthiophene in hydrocarbons |
| pvap | 33.26 | kPa | 373.10 | Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water |
| pvap | 111.40 | kPa | 413.15 | Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.42303e+01 |
| Coeff. B | -3.34101e+03 |
| Coeff. C | -5.96100e+01 |
| Temperature range (K), min. | 299.23 |
| Temperature range (K), max. | 434.21 |

# Datasets

## Mass density, kg/m3

| Temperature, K - Liquid | Pressure, kPa - Liquid | Mass density, kg/m3 - Liquid |
|---|---|---|
| 283.15 | 100.00 | 1003.44 |
| 288.15 | 100.00 | 998.47 |
| 293.15 | 100.00 | 993.45 |
| 298.15 | 100.00 | 988.39 |
| 303.15 | 100.00 | 983.42 |
| 308.15 | 100.00 | 978.38 |
| 313.15 | 100.00 | 973.34 |
| 318.15 | 100.00 | 968.32 |
| 323.15 | 100.00 | 963.21 |
| 328.15 | 100.00 | 958.12 |
| 333.15 | 100.00 | 952.99 |
| 338.15 | 100.00 | 947.86 |
| 283.15 | 2000.00 | 1004.84 |
| 288.15 | 2000.00 | 999.91 |
| 293.15 | 2000.00 | 994.92 |
| 298.15 | 2000.00 | 989.91 |
| 303.15 | 2000.00 | 984.97 |
| 308.15 | 2000.00 | 979.99 |
| 313.15 | 2000.00 | 975.0 |
| 318.15 | 2000.00 | 970.02 |

| | | |
|---|---|---|
| 323.15 | 2000.00 | 964.97 |
| 328.15 | 2000.00 | 959.94 |
| 333.15 | 2000.00 | 954.85 |
| 338.15 | 2000.00 | 949.78 |
| 283.15 | 5000.00 | 1007.0 |
| 288.15 | 5000.00 | 1002.13 |
| 293.15 | 5000.00 | 997.2 |
| 298.15 | 5000.00 | 992.26 |
| 303.15 | 5000.00 | 987.39 |
| 308.15 | 5000.00 | 982.48 |
| 313.15 | 5000.00 | 977.54 |
| 318.15 | 5000.00 | 972.64 |
| 323.15 | 5000.00 | 967.69 |
| 328.15 | 5000.00 | 962.71 |
| 333.15 | 5000.00 | 957.72 |
| 338.15 | 5000.00 | 952.72 |
| 283.15 | 7000.00 | 1008.42 |
| 288.15 | 7000.00 | 1003.59 |
| 293.15 | 7000.00 | 998.7 |
| 298.15 | 7000.00 | 993.8 |
| 303.15 | 7000.00 | 988.98 |
| 308.15 | 7000.00 | 984.11 |
| 313.15 | 7000.00 | 979.22 |
| 318.15 | 7000.00 | 974.36 |
| 323.15 | 7000.00 | 969.44 |
| 328.15 | 7000.00 | 964.53 |
| 333.15 | 7000.00 | 959.58 |
| 338.15 | 7000.00 | 954.65 |
| 283.15 | 10000.00 | 1010.51 |
| 288.15 | 10000.00 | 1005.73 |
| 293.15 | 10000.00 | 1000.9 |
| 298.15 | 10000.00 | 996.05 |
| 303.15 | 10000.00 | 991.3 |
| 308.15 | 10000.00 | 986.49 |
| 313.15 | 10000.00 | 981.68 |
| 318.15 | 10000.00 | 976.86 |
| 323.15 | 10000.00 | 972.03 |
| 328.15 | 10000.00 | 967.18 |
| 333.15 | 10000.00 | 962.31 |
| 338.15 | 10000.00 | 957.46 |
| 283.15 | 15000.00 | 1013.9 |
| 288.15 | 15000.00 | 1009.2 |
| 293.15 | 15000.00 | 1004.46 |
| 298.15 | 15000.00 | 999.7 |

| | | |
|---|---|---|
| 303.15 | 15000.00 | 995.04 |
| 308.15 | 15000.00 | 990.33 |
| 313.15 | 15000.00 | 985.61 |
| 318.15 | 15000.00 | 980.93 |
| 323.15 | 15000.00 | 976.2 |
| 328.15 | 15000.00 | 971.45 |
| 333.15 | 15000.00 | 966.72 |
| 338.15 | 15000.00 | 961.97 |
| 283.15 | 20000.00 | 1017.18 |
| 288.15 | 20000.00 | 1012.57 |
| 293.15 | 20000.00 | 1007.92 |
| 298.15 | 20000.00 | 1003.24 |
| 303.15 | 20000.00 | 998.67 |
| 308.15 | 20000.00 | 994.05 |
| 313.15 | 20000.00 | 989.42 |
| 318.15 | 20000.00 | 984.83 |
| 323.15 | 20000.00 | 980.22 |
| 328.15 | 20000.00 | 975.56 |
| 333.15 | 20000.00 | 970.93 |
| 338.15 | 20000.00 | 966.32 |
| 283.15 | 25000.00 | 1020.37 |
| 288.15 | 25000.00 | 1015.82 |
| 293.15 | 25000.00 | 1011.25 |
| 298.15 | 25000.00 | 1006.67 |
| 303.15 | 25000.00 | 1002.17 |
| 308.15 | 25000.00 | 997.63 |
| 313.15 | 25000.00 | 993.09 |
| 318.15 | 25000.00 | 988.58 |
| 323.15 | 25000.00 | 984.06 |
| 328.15 | 25000.00 | 979.5 |
| 333.15 | 25000.00 | 974.97 |
| 338.15 | 25000.00 | 970.44 |
| 283.15 | 30000.00 | 1023.45 |
| 288.15 | 30000.00 | 1018.97 |
| 293.15 | 30000.00 | 1014.49 |
| 298.15 | 30000.00 | 1009.97 |
| 303.15 | 30000.00 | 1005.54 |
| 308.15 | 30000.00 | 1001.09 |
| 313.15 | 30000.00 | 996.63 |
| 318.15 | 30000.00 | 992.22 |
| 323.15 | 30000.00 | 987.78 |
| 328.15 | 30000.00 | 983.31 |
| 333.15 | 30000.00 | 978.86 |
| 338.15 | 30000.00 | 974.41 |

| | | |
|---|---|---|
| 283.15 | 35000.00 | 1026.45 |
| 288.15 | 35000.00 | 1022.04 |
| 293.15 | 35000.00 | 1017.62 |
| 298.15 | 35000.00 | 1013.18 |
| 303.15 | 35000.00 | 1008.81 |
| 308.15 | 35000.00 | 1004.45 |
| 313.15 | 35000.00 | 1000.06 |
| 318.15 | 35000.00 | 995.71 |
| 323.15 | 35000.00 | 991.35 |
| 328.15 | 35000.00 | 986.98 |
| 333.15 | 35000.00 | 982.61 |
| 338.15 | 35000.00 | 978.26 |
| 283.15 | 40000.00 | 1029.36 |
| 288.15 | 40000.00 | 1025.03 |
| 293.15 | 40000.00 | 1020.67 |
| 298.15 | 40000.00 | 1016.3 |
| 303.15 | 40000.00 | 1012.0 |
| 308.15 | 40000.00 | 1007.68 |
| 313.15 | 40000.00 | 1003.38 |
| 318.15 | 40000.00 | 999.11 |
| 323.15 | 40000.00 | 994.81 |
| 328.15 | 40000.00 | 990.51 |
| 333.15 | 40000.00 | 986.22 |
| 338.15 | 40000.00 | 981.96 |
| 283.15 | 45000.00 | 1032.2 |
| 288.15 | 45000.00 | 1027.9 |
| 293.15 | 45000.00 | 1023.61 |
| 298.15 | 45000.00 | 1019.31 |
| 303.15 | 45000.00 | 1015.07 |
| 308.15 | 45000.00 | 1010.84 |
| 313.15 | 45000.00 | 1006.6 |
| 318.15 | 45000.00 | 1002.39 |
| 323.15 | 45000.00 | 998.17 |
| 328.15 | 45000.00 | 993.94 |
| 333.15 | 45000.00 | 989.73 |
| 338.15 | 45000.00 | 985.53 |
| 283.15 | 50000.00 | 1034.96 |
| 288.15 | 50000.00 | 1030.72 |
| 293.15 | 50000.00 | 1026.49 |
| 298.15 | 50000.00 | 1022.24 |
| 303.15 | 50000.00 | 1018.07 |
| 308.15 | 50000.00 | 1013.88 |
| 313.15 | 50000.00 | 1009.71 |
| 318.15 | 50000.00 | 1005.57 |

| | | |
|---|---|---|
| 323.15 | 50000.00 | 1001.41 |
| 328.15 | 50000.00 | 997.24 |
| 333.15 | 50000.00 | 993.09 |
| 338.15 | 50000.00 | 988.98 |
| 283.15 | 55000.00 | 1037.65 |
| 288.15 | 55000.00 | 1033.47 |
| 293.15 | 55000.00 | 1029.29 |
| 298.15 | 55000.00 | 1025.1 |
| 303.15 | 55000.00 | 1020.99 |
| 308.15 | 55000.00 | 1016.86 |
| 313.15 | 55000.00 | 1012.75 |
| 318.15 | 55000.00 | 1008.66 |
| 323.15 | 55000.00 | 1004.56 |
| 328.15 | 55000.00 | 1000.47 |
| 333.15 | 55000.00 | 996.39 |
| 338.15 | 55000.00 | 992.31 |
| 283.15 | 60000.00 | 1040.28 |
| 288.15 | 60000.00 | 1036.14 |
| 293.15 | 60000.00 | 1032.01 |
| 298.15 | 60000.00 | 1027.87 |
| 303.15 | 60000.00 | 1023.81 |
| 308.15 | 60000.00 | 1019.74 |
| 313.15 | 60000.00 | 1015.69 |
| 318.15 | 60000.00 | 1011.66 |
| 323.15 | 60000.00 | 1007.62 |
| 328.15 | 60000.00 | 1003.58 |
| 333.15 | 60000.00 | 999.56 |
| 338.15 | 60000.00 | 995.56 |
| 283.15 | 65000.00 | 1042.84 |
| 288.15 | 65000.00 | 1038.73 |
| 293.15 | 65000.00 | 1034.65 |
| 298.15 | 65000.00 | 1030.59 |
| 303.15 | 65000.00 | 1026.56 |
| 308.15 | 65000.00 | 1022.56 |
| 313.15 | 65000.00 | 1018.54 |
| 318.15 | 65000.00 | 1014.56 |
| 323.15 | 65000.00 | 1010.59 |
| 328.15 | 65000.00 | 1006.6 |
| 333.15 | 65000.00 | 1002.62 |
| 338.15 | 65000.00 | 998.71 |

Reference *https://www.doi.org/10.1021/acs.jced.8b00153*

# Sources

| | |
|---|---|
| **Phase equilibria of three binary systems containing 2,5-dimethylthiophene and 2-ethylthiophene in hydrocarbons:** | https://www.doi.org/10.1016/j.fluid.2015.09.030 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water:** | https://www.doi.org/10.1021/je050473r |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C872559&Units=SI |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Isobaric vapor-liquid equilibrium for binary systemof 2-ethylthiophene + n-octane at 101.33 kPa:** | https://www.doi.org/10.1016/j.fluid.2014.07.010 |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Comparative Study of the Thermophysical Properties of 2-Ethylthiophene and 2-Ethylfuran:** | https://www.doi.org/10.1021/acs.jced.8b00153 |

# Legend

| | |
|---|---|
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pvap:** | Vapor pressure |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |