# 3-(Thiiran-2-yl)propanenitrile

**Other names:** 3,4-Epoxythiobutyl cyanide
**Inchi:** InChI=1S/C5H7NS/c6-3-1-2-5-4-7-5/h5H,1-2,4H2
**InchiKey:** ZAGXORSINWAUSP-UHFFFAOYSA-N
**Formula:** C5H7NS
**SMILES:** N#CCCC1CS1
**Mol. weight [g/mol]:** 113.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 12.00 | kJ/mol | Joback Method |
| logp | 1.406 | | Crippen Method |
| mcvol | 88.180 | ml/mol | McGowan Method |
| rinpol | 1086.00 | | NIST Webbook |
| rinpol | 1124.00 | | NIST Webbook |
| rinpol | 1122.50 | | NIST Webbook |
| rinpol | 1075.00 | | NIST Webbook |
| rinpol | 1086.00 | | NIST Webbook |
| rinpol | 1122.50 | | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 173.95 | J/mol×K | 470.45 | Joback Method |
| cpg | 182.86 | J/mol×K | 507.49 | Joback Method |
| cpg | 191.15 | J/mol×K | 544.53 | Joback Method |
| cpg | 198.86 | J/mol×K | 581.57 | Joback Method |
| cpg | 206.03 | J/mol×K | 618.61 | Joback Method |
| cpg | 212.72 | J/mol×K | 655.65 | Joback Method |
| cpg | 218.97 | J/mol×K | 692.69 | Joback Method |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C54096456&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |