

trans-3-ethyl-5-methyl-1,2-dithiolan-4-one

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| Inchi: | InChI=1S/C6H10OS2/c1-3-5-6(7)4(2)8-9-5/h4-5H,3H2,1-2H3 |
| InchiKey: | MMXLOINISPYVFC-UHFFFAOYSA-N |
| Formula: | C6H10OS2 |
| SMILES: | CCC1SSC(C)C1=O |
| Mol. weight [g/mol]: | 162.27 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -14.39 | kJ/mol | Joback Method |
| hf | -174.21 | kJ/mol | Joback Method |
| hfus | 13.13 | kJ/mol | Joback Method |
| hvap | 44.77 | kJ/mol | Joback Method |
| log10ws | -2.49 | | Crippen Method |
| logp | 2.118 | | Crippen Method |
| mvol | 118.810 | ml/mol | McGowan Method |
| pc | 3791.65 | kPa | Joback Method |
| ripol | 1669.00 | | NIST Webbook |
| ripol | 1669.00 | | NIST Webbook |
| tb | 510.77 | K | Joback Method |
| tc | 758.59 | K | Joback Method |
| tf | 399.16 | K | Joback Method |
| vc | 0.410 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 251.54 | J/mol×K | 510.77 | Joback Method |
| cpg | 265.61 | J/mol×K | 552.07 | Joback Method |
| cpg | 278.98 | J/mol×K | 593.38 | Joback Method |
| cpg | 291.62 | J/mol×K | 634.68 | Joback Method |
| cpg | 303.54 | J/mol×K | 675.98 | Joback Method |
| cpg | 314.72 | J/mol×K | 717.28 | Joback Method |
| cpg | 325.15 | J/mol×K | 758.59 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=R432676&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 |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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