

4(E),8(Z)-Matricaria lactone

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|-----------------------------|--|
| Inchi: | InChI=1S/C10H10O2/c1-2-3-4-5-6-9-7-8-10(11)12-9/h2-3,6H,7-8H2,1H3/b3-2-,9-6+ |
| InchiKey: | NUPAKTQITFGCSA-NRNOEJAFSA-N |
| Formula: | C10H10O2 |
| SMILES: | CC=CC#CC=C1CCC(=O)O1 |
| Mol. weight [g/mol]: | 162.19 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 197.35 | kJ/mol | Joback Method |
| hf | 26.94 | kJ/mol | Joback Method |
| hfus | 25.66 | kJ/mol | Joback Method |
| hvap | 50.07 | kJ/mol | Joback Method |
| log10ws | -2.76 | | Crippen Method |
| logp | 1.787 | | Crippen Method |
| mvol | 131.140 | ml/mol | McGowan Method |
| pc | 3468.36 | kPa | Joback Method |
| rinpol | 1490.00 | | NIST Webbook |
| rinpol | 1490.00 | | NIST Webbook |
| tb | 562.72 | K | Joback Method |
| tc | 813.11 | K | Joback Method |
| tf | 423.77 | K | Joback Method |
| vc | 0.490 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 294.43 | J/mol×K | 562.72 | Joback Method |
| cpg | 308.76 | J/mol×K | 604.45 | Joback Method |
| cpg | 322.18 | J/mol×K | 646.18 | Joback Method |
| cpg | 334.75 | J/mol×K | 687.92 | Joback Method |
| cpg | 346.48 | J/mol×K | 729.65 | Joback Method |
| cpg | 357.42 | J/mol×K | 771.38 | Joback Method |
| cpg | 367.60 | J/mol×K | 813.11 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R634570&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|-----------------|---|
| 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 |
| hvp: | 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 |
| rinp: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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