

4-Methoxycinnamotrile,c&t

| | |
|-----------------------------|---|
| Other names: | 4-Methoxycinnamotrile cis + trans 2-Propenenitrile, 3-(4-methoxyphenyl)- Cinnamotrile, p-methoxy- p-Methoxycinnamotrile cis,trans-4-methoxycinnamotrile |
| Inchi: | InChI=1S/C10H9NO/c1-12-10-6-4-9(5-7-10)3-2-8-11/h2-7H,1H3/b3-2+ |
| InchiKey: | CNBCNHHPIBKYBO-NSCUHMNNSA-N |
| Formula: | C10H9NO |
| SMILES: | COc1ccc(C=CC#N)cc1 |
| Mol. weight [g/mol]: | 159.18 |
| CAS: | 28446-68-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 244.50 | kJ/mol | Joback Method |
| hf | 125.21 | kJ/mol | Joback Method |
| hfus | 18.20 | kJ/mol | Joback Method |
| hvap | 53.64 | kJ/mol | Joback Method |
| log10ws | -2.70 | | Crippen Method |
| logp | 2.232 | | Crippen Method |
| mcvol | 130.950 | ml/mol | McGowan Method |
| pc | 2915.53 | kPa | Joback Method |
| tb | 588.52 | K | Joback Method |
| tc | 820.00 | K | Joback Method |
| tf | 323.54 | K | Joback Method |
| vc | 0.511 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 290.31 | J/mol×K | 588.52 | Joback Method |
| cpg | 301.65 | J/mol×K | 627.10 | Joback Method |
| cpg | 312.25 | J/mol×K | 665.68 | Joback Method |
| cpg | 322.15 | J/mol×K | 704.26 | Joback Method |

| | | | | |
|-----|--------|---------|--------|---------------|
| cpg | 331.37 | J/mol×K | 742.84 | Joback Method |
| cpg | 339.95 | J/mol×K | 781.42 | Joback Method |
| cpg | 347.93 | J/mol×K | 820.00 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C28446686&Units=SI |

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 |
| 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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/79-769-2/4-Methoxycinnamotrile-candt.pdf>

Generated by Cheméo on 2024-04-26 09:30:39.662637493 +0000 UTC m=+16413088.583214808.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.