

2-Trifluoromethylbenzoic acid, ethyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C10H9F3O2/c1-2-15-9(14)7-5-3-4-6-8(7)10(11,12)13/h3-6H,2H2,1H3 |
| InchiKey: | BQLMZZVRHPZRQBQ-UHFFFAOYSA-N |
| Formula: | C10H9F3O2 |
| SMILES: | CCOC(=O)c1ccccc1C(F)(F)F |
| Mol. weight [g/mol]: | 218.17 |
| CAS: | 577-62-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -679.41 | kJ/mol | Joback Method |
| hf | -866.55 | kJ/mol | Joback Method |
| hfus | 19.92 | kJ/mol | Joback Method |
| hvap | 46.20 | kJ/mol | Joback Method |
| log10ws | -3.24 | | Crippen Method |
| logp | 2.882 | | Crippen Method |
| mcvol | 140.750 | ml/mol | McGowan Method |
| pc | 2679.08 | kPa | Joback Method |
| tb | 530.73 | K | Joback Method |
| tc | 726.25 | K | Joback Method |
| tf | 317.75 | K | Joback Method |
| vc | 0.554 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 328.54 | J/molxK | 530.73 | Joback Method |
| cpg | 340.77 | J/molxK | 563.32 | Joback Method |
| cpg | 352.26 | J/molxK | 595.90 | Joback Method |
| cpg | 363.03 | J/molxK | 628.49 | Joback Method |
| cpg | 373.10 | J/molxK | 661.08 | Joback Method |
| cpg | 382.52 | J/molxK | 693.66 | Joback Method |
| cpg | 391.31 | J/molxK | 726.25 | 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=C577628&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 |
| h vap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| m cvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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