

Carbonic acid, 2-methoxyethyl 3,5-difluorophenyl ester

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|----------------------|---|
| Inchi: | InChI=1S/C10H10F2O4/c1-14-2-3-15-10(13)16-9-5-7(11)4-8(12)6-9/h4-6H,2-3H2,1H3 |
| InchiKey: | KMEJNIVAYBMZSV-UHFFFAOYSA-N |
| Formula: | C10H10F2O4 |
| SMILES: | COCCOC(=O)Oc1cc(F)cc(F)c1 |
| Mol. weight [g/mol]: | 232.18 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -707.07 | kJ/mol | Joback Method |
| hf | -937.60 | kJ/mol | Joback Method |
| hfus | 26.24 | kJ/mol | Joback Method |
| hvap | 53.80 | kJ/mol | Joback Method |
| log10ws | -2.44 | | Crippen Method |
| logp | 2.127 | | Crippen Method |
| mcvol | 150.720 | ml/mol | McGowan Method |
| pc | 2616.41 | kPa | Joback Method |
| rinqol | 1379.00 | | NIST Webbook |
| tb | 584.51 | K | Joback Method |
| tc | 776.19 | K | Joback Method |
| tf | 371.72 | K | Joback Method |
| vc | 0.584 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 363.63 | J/molxK | 584.51 | Joback Method |
| cpg | 375.08 | J/molxK | 616.46 | Joback Method |
| cpg | 386.04 | J/molxK | 648.40 | Joback Method |
| cpg | 396.48 | J/molxK | 680.35 | Joback Method |
| cpg | 406.39 | J/molxK | 712.30 | Joback Method |
| cpg | 415.76 | J/molxK | 744.24 | Joback Method |
| cpg | 424.57 | J/molxK | 776.19 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U357866&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| hvac: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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