

2-(2,2,3,3,3-Pentafluoropropanoyl)oxyethyl 2,2,3,3,3-pentafluoropropanoate

Other names: Ethylene glycol, bis(pentafluoropropionate)

Inchi: InChI=1S/C8H4F10O4/c9-5(10,7(13,14)15)3(19)21-1-2-22-4(20)6(11,12)8(16,17)18/h1-2

InchiKey: CNMNDNGVVAWZNK-UHFFFAOYSA-N

Formula: C8H4F10O4

SMILES: O=C(OCCOC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 354.10

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -2388.10 | kJ/mol | Joback Method |
| hf | -2694.15 | kJ/mol | Joback Method |
| hfus | 23.19 | kJ/mol | Joback Method |
| hvap | 38.36 | kJ/mol | Joback Method |
| log10ws | -2.85 | | Crippen Method |
| logp | 2.468 | | Crippen Method |
| mcvol | 156.160 | ml/mol | McGowan Method |
| pc | 1944.08 | kPa | Joback Method |
| rinpola | 844.60 | | NIST Webbook |
| tb | 514.80 | K | Joback Method |
| tc | 661.80 | K | Joback Method |
| tf | 339.82 | K | Joback Method |
| vc | 0.667 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 418.50 | J/mol×K | 514.80 | Joback Method |
| cpg | 428.18 | J/mol×K | 539.30 | Joback Method |
| cpg | 437.24 | J/mol×K | 563.80 | Joback Method |
| cpg | 445.70 | J/mol×K | 588.30 | Joback Method |
| cpg | 453.60 | J/mol×K | 612.80 | Joback Method |
| cpg | 460.95 | J/mol×K | 637.30 | Joback Method |
| cpg | 467.79 | J/mol×K | 661.80 | 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=U352001&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |

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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