

n-Decanal, o-[(pentafluorophenyl)methyl]oxime

Other names: Decanal, PFBO # 2
Inchi: InChI=1S/C17H22F5NO/c1-2-3-4-5-6-7-8-9-10-23-24-11-12-13(18)15(20)17(22)16(21)14
InchiKey: NUGDFCWVLOJWOP-UHFFFAOYSA-N
Formula: C17H22F5NO
SMILES: CCCCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 351.35

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|--------|----------------|
| hf | -1245.58 | kJ/mol | Joback Method |
| hvap | 60.66 | kJ/mol | Joback Method |
| log10ws | -7.44 | | Crippen Method |
| logp | 6.025 | | Crippen Method |
| mcvol | 247.030 | ml/mol | McGowan Method |
| pc | 1156.14 | kPa | Joback Method |
| ripol | 2143.00 | | NIST Webbook |
| ripol | 2143.00 | | NIST Webbook |
| tb | 735.39 | K | Joback Method |
| tc | 911.89 | K | 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=U288101&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf: Enthalpy of formation at standard conditions

| | |
|---------------------------------------|---|
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀w_s: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mc_{vol}: | McGowan's characteristic volume |
| p_c: | Critical Pressure |
| ri_{pol}: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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