# «alpha»-Hydroxybehenic acid, HFB-Me

**Inchi:** InChI=1S/C27H45F7O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23(3
**InchiKey:** JBLKXFRSPSLDPU-UHFFFAOYSA-N
**Formula:** C27H45F7O4
**SMILES:** CCCCCCCCCCCCCCCCCCCCCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)OC
**Mol. weight [g/mol]:** 566.63

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1648.97 | kJ/mol | Joback Method |
| hf | -2494.51 | kJ/mol | Joback Method |
| hfus | 67.05 | kJ/mol | Joback Method |
| hvap | 84.01 | kJ/mol | Joback Method |
| log10ws | -10.25 | | Crippen Method |
| logp | 9.336 | | Crippen Method |
| mcvol | 418.560 | ml/mol | McGowan Method |
| pc | 635.12 | kPa | Joback Method |
| rinpol | 2564.00 | | NIST Webbook |
| rinpol | 2564.00 | | NIST Webbook |
| tb | 954.50 | K | Joback Method |
| tc | 1192.73 | K | Joback Method |
| tf | 534.76 | K | Joback Method |
| vc | 1.683 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1456.79 | J/mol×K | 954.50 | Joback Method |
| cpg | 1478.70 | J/mol×K | 994.20 | Joback Method |
| cpg | 1498.99 | J/mol×K | 1033.91 | Joback Method |
| cpg | 1517.81 | J/mol×K | 1073.61 | Joback Method |
| cpg | 1535.33 | J/mol×K | 1113.32 | Joback Method |
| cpg | 1551.72 | J/mol×K | 1153.02 | Joback Method |
| cpg | 1567.14 | J/mol×K | 1192.73 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R134228&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# 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 |
| **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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