# Pentosyl «beta»-D-glucopyranoside of methyl salicylate, isomer # 1, TFA

**Inchi:** InChI=1S/C22H14F12O12/c1-40-13(35)7-4-2-3-5-8(7)42-14-12(46-18(39)22(32,33)34)11

**InchiKey:** NWJNOOFMDOXMLR-ZAOAHOKWSA-N

**Formula:** C22H14F12O12

**SMILES:** COC(=O)c1ccccc1OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1

**Mol. weight [g/mol]:** 698.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 72.91 | kJ/mol | Joback Method |
| log10ws | -6.20 | | Cheméo Relay (1.0) |
| logp | 3.105 | | Crippen Method |
| mcvol | 356.400 | ml/mol | McGowan Method |
| rinpol | 2288.00 | | NIST Webbook |
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## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1230.27 | J/mol×K | 1144.43 | Joback Method |
| cpg | 1230.21 | J/mol×K | 1192.42 | Joback Method |
| cpg | 1227.04 | J/mol×K | 1240.41 | Joback Method |
| cpg | 1220.82 | J/mol×K | 1288.39 | Joback Method |
| cpg | 1211.64 | J/mol×K | 1336.38 | Joback Method |
| cpg | 1199.58 | J/mol×K | 1384.37 | Joback Method |
| cpg | 1184.71 | J/mol×K | 1432.36 | Joback Method |

## Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R330486&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |