# 1,4-Di-t-butylperoxy pyromellitate

**Inchi:** InChI=1S/C18H22O10/c1-17(2,3)27-25-15(23)11-7-10(14(21)22)12(8-9(11)13(19)20)16(
**InchiKey:** MXFZJFCNTQTGHU-UHFFFAOYSA-N
**Formula:** C18H22O10
**SMILES:** CC(C)(C)OOC(=O)c1cc(C(=O)O)c(C(=O)OOC(C)(C)C)cc1C(=O)O
**Mol. weight [g/mol]:** 398.36
**CAS:** 82234-37-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -8566.10 ± 6.00 | kJ/mol | NIST Webbook |
| gf | -1019.44 | kJ/mol | Joback Method |
| hf | -1513.89 | kJ/mol | Joback Method |
| hfs | -1661.80 ± 6.00 | kJ/mol | NIST Webbook |
| hfus | 39.75 | kJ/mol | Joback Method |
| hvap | 127.31 | kJ/mol | Joback Method |
| log10ws | -4.97 | | Crippen Method |
| logp | 2.857 | | Crippen Method |
| mcvol | 282.220 | ml/mol | McGowan Method |
| pc | 1968.30 | kPa | Joback Method |
| tb | 1135.92 | K | Joback Method |
| tc | 1396.14 | K | Joback Method |
| tf | 771.72 | K | Joback Method |
| vc | 1.048 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 916.47 | J/mol×K | 1135.92 | Joback Method |
| cpg | 921.08 | J/mol×K | 1179.29 | Joback Method |
| cpg | 923.99 | J/mol×K | 1222.66 | Joback Method |
| cpg | 925.22 | J/mol×K | 1266.03 | Joback Method |
| cpg | 924.82 | J/mol×K | 1309.40 | Joback Method |
| cpg | 922.80 | J/mol×K | 1352.77 | Joback Method |
| cpg | 919.21 | J/mol×K | 1396.14 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000046 | Pa×s | 771.72 | Joback Method |
| dvisc | 0.0000023 | Pa×s | 832.42 | Joback Method |
| dvisc | 0.0000013 | Pa×s | 893.12 | Joback Method |
| dvisc | 0.0000008 | Pa×s | 953.82 | Joback Method |
| dvisc | 0.0000005 | Pa×s | 1014.52 | Joback Method |
| dvisc | 0.0000003 | Pa×s | 1075.22 | Joback Method |
| dvisc | 0.0000002 | Pa×s | 1135.92 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C82234375&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

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

Latest version available from:
https://www.chemeo.com/cid/78-220-1/1-4-Di-t-butylperoxy-pyromellitate.pdf
Generated by Cheméo on 2024-10-12 05:57:42.405959179 +0000 UTC m=+3293525.042928428.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.