# (-)-Norepinephrine, N,O,O',O''-tetrakis(pentafluoropropionyl)-

**Inchi:** InChI=1S/C20H7F20NO7/c21-13(22,17(29,30)31)9(42)41-4-8(48-12(45)16(27,28)20(38,3

**InchiKey:** BLOMCUYCULPLFG-UHFFFAOYSA-N

**Formula:** C20H7F20NO7

**SMILES:** O=C(NCC(OC(=O)C(F)(F)C(F)(F)F)c1ccc(OC(=O)C(F)(F)C(F)(F)F)c(OC(=O)C(F)(F)C(F)

**Mol. weight [g/mol]:** 753.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -4406.54 | kJ/mol | Joback Method |
| hf | -5033.53 | kJ/mol | Joback Method |
| hfus | 54.64 | kJ/mol | Joback Method |
| hvap | 77.27 | kJ/mol | Joback Method |
| log10ws | -8.44 | | Crippen Method |
| logp | 5.988 | | Crippen Method |
| mcvol | 338.170 | ml/mol | McGowan Method |
| pc | 884.19 | kPa | Joback Method |
| rinpol | 1520.00 | | NIST Webbook |
| rinpol | 1520.00 | | NIST Webbook |
| tb | 985.67 | K | Joback Method |
| tc | 1231.36 | K | Joback Method |
| tf | 701.85 | K | Joback Method |
| vc | 1.427 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1125.64 | J/mol×K | 985.67 | Joback Method |
| cpg | 1134.18 | J/mol×K | 1026.62 | Joback Method |
| cpg | 1142.20 | J/mol×K | 1067.57 | Joback Method |
| cpg | 1149.99 | J/mol×K | 1108.51 | Joback Method |
| cpg | 1157.84 | J/mol×K | 1149.46 | Joback Method |
| cpg | 1166.04 | J/mol×K | 1190.41 | Joback Method |
| cpg | 1174.87 | J/mol×K | 1231.36 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U375716&Units=SI |

# 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 |