# Sebacic acid, 3-nitro-4-fluorobenzyl propyl ester

**Inchi:** InChI=1S/C20H28FNO6/c1-2-13-27-19(23)9-7-5-3-4-6-8-10-20(24)28-15-16-11-12-17(21

**InchiKey:** FNNJYXYVZVQBTL-UHFFFAOYSA-N

**Formula:** C20H28FNO6

**SMILES:** CCCOC(=O)CCCCCCCCC(=O)OCc1ccc(F)c([N+](=O)[O-])c1

**Mol. weight [g/mol]:** 397.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -416.43 | kJ/mol | Joback Method |
| hf | -939.01 | kJ/mol | Joback Method |
| hfus | 60.83 | kJ/mol | Joback Method |
| hvap | 97.80 | kJ/mol | Joback Method |
| log10ws | -6.50 | | Crippen Method |
| logp | 4.851 | | Crippen Method |
| mcvol | 302.970 | ml/mol | McGowan Method |
| pc | 1295.79 | kPa | Joback Method |
| rinpol | 2889.00 | | NIST Webbook |
| rinpol | 2889.00 | | NIST Webbook |
| tb | 997.33 | K | Joback Method |
| tc | 1222.24 | K | Joback Method |
| tf | 655.14 | K | Joback Method |
| vc | 1.196 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 993.96 | J/mol×K | 997.33 | Joback Method |
| cpg | 1006.19 | J/mol×K | 1034.81 | Joback Method |
| cpg | 1017.04 | J/mol×K | 1072.30 | Joback Method |
| cpg | 1026.57 | J/mol×K | 1109.78 | Joback Method |
| cpg | 1034.79 | J/mol×K | 1147.27 | Joback Method |
| cpg | 1041.75 | J/mol×K | 1184.75 | Joback Method |
| cpg | 1047.46 | J/mol×K | 1222.24 | 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=U380694&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 |