# 3-Methoxy-5-nitrobenzotrifluoride

**Inchi:** InChI=1S/C8H6F3NO3/c1-15-7-3-5(8(9,10)11)2-6(4-7)12(13)14/h2-4H,1H3
**InchiKey:** NCPVPJVRLLHBEL-UHFFFAOYSA-N
**Formula:** C8H6F3NO3
**SMILES:** COc1cc([N+](=O)[O-])cc(C(F)(F)F)c1
**Mol. weight [g/mol]:** 221.13
**CAS:** 328-79-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -541.41 | kJ/mol | Joback Method |
| hf | -734.92 | kJ/mol | Joback Method |
| hfus | 24.11 | kJ/mol | Joback Method |
| hvap | 52.26 | kJ/mol | Joback Method |
| log10ws | -3.35 | | Crippen Method |
| logp | 2.622 | | Crippen Method |
| mcvol | 128.420 | ml/mol | McGowan Method |
| pc | 3065.95 | kPa | Joback Method |
| tb | 587.92 | K | Joback Method |
| tc | 809.18 | K | Joback Method |
| tf | 401.41 | K | Joback Method |
| vc | 0.518 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 315.13 | J/mol×K | 587.92 | Joback Method |
| cpg | 325.67 | J/mol×K | 624.80 | Joback Method |
| cpg | 335.44 | J/mol×K | 661.67 | Joback Method |
| cpg | 344.46 | J/mol×K | 698.55 | Joback Method |
| cpg | 352.78 | J/mol×K | 735.42 | Joback Method |
| cpg | 360.43 | J/mol×K | 772.30 | Joback Method |
| cpg | 367.44 | J/mol×K | 809.18 | Joback Method |

# Sources

| | |
|---|---|
| **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=C328790&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |