# 1-nitro-3-methylbutane

**Other names:** Butane, 3-methyl-1-nitro-
Nitro-3-methylbutane
3-methyl-1-nitrobutane
**Inchi:** InChI=1S/C5H11NO2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3
**InchiKey:** FEJLPMVSVDSKHJ-UHFFFAOYSA-N
**Formula:** C5H11NO2
**SMILES:** CC(C)CC[N+](=O)[O-]
**Mol. weight [g/mol]:** 117.15
**CAS:** 627-67-8

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 24.33 | kJ/mol | Joback Method |
| hf | -162.57 | kJ/mol | Joback Method |
| hfus | 16.54 | kJ/mol | Joback Method |
| hvap | 42.93 | kJ/mol | Joback Method |
| log10ws | -1.76 | | Crippen Method |
| logp | 1.309 | | Crippen Method |
| mcvol | 98.730 | ml/mol | McGowan Method |
| pc | 3551.53 | kPa | Joback Method |
| rinpol | 856.00 | | NIST Webbook |
| rinpol | 887.00 | | NIST Webbook |
| ripol | 1308.00 | | NIST Webbook |
| ripol | 1339.00 | | NIST Webbook |
| ripol | 1317.00 | | NIST Webbook |
| ripol | 1308.00 | | NIST Webbook |
| tb | 465.20 | K | Joback Method |
| tc | 674.41 | K | Joback Method |
| tf | 274.72 | K | Joback Method |
| vc | 0.392 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 209.31 | J/mol×K | 465.20 | Joback Method |
| cpg | 220.22 | J/mol×K | 500.07 | Joback Method |
| cpg | 230.58 | J/mol×K | 534.94 | Joback Method |
| cpg | 240.40 | J/mol×K | 569.81 | Joback Method |
| cpg | 249.70 | J/mol×K | 604.68 | Joback Method |
| cpg | 258.50 | J/mol×K | 639.54 | Joback Method |
| cpg | 266.81 | J/mol×K | 674.41 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C627678&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 |

# Legend

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|---|---|
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |