# Butane, 2,3-dimethyl-2-nitro-

**Inchi:** InChI=1S/C6H13NO2/c1-5(2)6(3,4)7(8)9/h5H,1-4H3
**InchiKey:** PKOVWKGRNZGQHY-UHFFFAOYSA-N
**Formula:** C6H13NO2
**SMILES:** CC(C)C(C)(C)[N+](=O)[O-]
**Mol. weight [g/mol]:** 131.17
**CAS:** 34075-28-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 35.59 | kJ/mol | Joback Method |
| hf | -191.96 | kJ/mol | Joback Method |
| hfus | 11.72 | kJ/mol | Joback Method |
| hvap | 43.86 | kJ/mol | Joback Method |
| log10ws | -2.29 | | Crippen Method |
| logp | 1.698 | | Crippen Method |
| mcvol | 112.820 | ml/mol | McGowan Method |
| pc | 3246.73 | kPa | Joback Method |
| tb | 446.65 ± 2.00 | K | NIST Webbook |
| tc | 705.02 | K | Joback Method |
| tf | 302.40 ± 1.00 | K | NIST Webbook |
| vc | 0.436 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 253.60 | J/mol×K | 484.85 | Joback Method |
| cpg | 266.82 | J/mol×K | 521.55 | Joback Method |
| cpg | 279.19 | J/mol×K | 558.24 | Joback Method |
| cpg | 290.74 | J/mol×K | 594.94 | Joback Method |
| cpg | 301.53 | J/mol×K | 631.63 | Joback Method |
| cpg | 311.58 | J/mol×K | 668.33 | Joback Method |
| cpg | 320.96 | J/mol×K | 705.02 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C34075280&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

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