# Anisole, 2-sec-butyl-4,6-dinitro-

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|---|---|
| **Other names:** | DNBPME |
| | 2,4-Dinitro-6-sec-butylphenol methyl ether |
| | Dinoseb, methyl ether |
| | Dinoseb methyl ester |
| | Phenol, 2-(1-methylpropyl)-4,6-dinitro-, methylated |
| | Phenol, 2-(1-methylpropyl), 4,6-dinitro, methyl ether |
| **Inchi:** | InChI=1S/C11H14N2O5/c1-4-7(2)9-5-8(12(14)15)6-10(13(16)17)11(9)18-3/h5-7H,4H2,1- |
| **InchiKey:** | UVYHORVGKZXEMP-UHFFFAOYSA-N |
| **Formula:** | C11H14N2O5 |
| **SMILES:** | CCC(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC |
| **Mol. weight [g/mol]:** | 254.24 |
| **CAS:** | 6099-79-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 88.92 | kJ/mol | Joback Method |
| hf | -227.27 | kJ/mol | Joback Method |
| hfus | 37.51 | kJ/mol | Joback Method |
| hvap | 79.55 | kJ/mol | Joback Method |
| log10ws | -4.50 | | Crippen Method |
| logp | 3.025 | | Crippen Method |
| mcvol | 182.800 | ml/mol | McGowan Method |
| pc | 2568.89 | kPa | Joback Method |
| tb | 818.36 | K | Joback Method |
| tc | 1069.43 | K | Joback Method |
| tf | 572.16 | K | Joback Method |
| vc | 0.720 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 526.31 | J/mol×K | 818.36 | Joback Method |
| cpg | 538.33 | J/mol×K | 860.20 | Joback Method |
| cpg | 549.25 | J/mol×K | 902.05 | Joback Method |

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|---|---|---|---|---|
| cpg | 559.10 | J/mol×K | 943.89 | Joback Method |
| cpg | 567.91 | J/mol×K | 985.74 | Joback Method |
| cpg | 575.70 | J/mol×K | 1027.58 | Joback Method |
| cpg | 582.49 | J/mol×K | 1069.43 | Joback Method |

# Sources

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|---|---|
| **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=C6099792&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |