# 4-TERT-BUTYL-3-METHOXY-2,6-DINITROTOLUEN

**Other names:** 1-(1,1-Dimethylethyl)-2-methoxy-4-methyl-3,5-dinitrobenzene
1-Methyl-4-t-butyl-3-methoxy-2,6-dinitrobenzene
1-Methyl-4-tert-butyl-3-methoxy-2,6-dinitrobenzene
2,4-Dinitro-3-methyl-6-tert-butylanisole
2,6-Dinitro-3-methoxy-4-tert-butyltoluene
2-tert-Butyl-4,6-dinitro-5-methylanisole
4-tert-Butyl-2,6-dinitro-3-methoxytoluene
4-tert-Butyl-3-methoxy-2,6-dinitrotoluene
5-t-Butyl-1,3-dinitro-4-methoxy-2-methylbenzene
6-t-Butyl-3-methyl-2,4-dinitroanisole
6-tert-Butyl-3-Methyl-2,4-dinitroanisol
6-tert-Butyl-3-methyl-2,4-dinitroanisole
Amber musk
Ambrette musk
Anisole, 6-t-butyl-3-methyl-2,4-dinitro-
Anisole, 6-tert-butyl-3-methyl-2,4-dinitro-
Artificial musk ambrette
Benzene, 1-(1,1-dimethylethyl)-2-methoxy-4-methyl-3,5-dinitro-
Musk amberette
Musk ambrette
NSC 46122
Synthetic musk ambrette

**Inchi:** InChI=1S/C12H16N2O5/c1-7-9(13(15)16)6-8(12(2,3)4)11(19-5)10(7)14(17)18/h6H,1-5H3

**InchiKey:** SUAUILGSCPYJCS-UHFFFAOYSA-N

**Formula:** C12H16N2O5

**SMILES:** COc1c(C(C)(C)C)cc([N+](=O)[O-])c(C)c1[N+](=O)[O-]

**Mol. weight [g/mol]:** 268.27

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -178.68 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 35.82 | kJ/mol | Joback Method |
| hvap | 82.16 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.77 | eV | Cheméo Relay (1.0) |
| log10ws | -4.49 | | Cheméo Relay (1.0) |
| logp | 3.118 | | Crippen Method |

| | | | |
|---|---|---|---|
| mcvol | 196.890 | ml/mol | McGowan Method |
| tf | 370.28 | K | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 580.04 | J/mol×K | 843.43 | Joback Method |
| cpg | 592.38 | J/mol×K | 885.94 | Joback Method |
| cpg | 603.61 | J/mol×K | 928.46 | Joback Method |
| cpg | 613.79 | J/mol×K | 970.97 | Joback Method |
| cpg | 622.97 | J/mol×K | 1013.49 | Joback Method |
| cpg | 631.20 | J/mol×K | 1056.00 | Joback Method |
| cpg | 638.53 | J/mol×K | 1098.52 | Joback Method |
| hsubt | 102.90 | kJ/mol | 323.00 | NIST Webbook |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C83669&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**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
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hsubt:** Enthalpy of sublimation at a given temperature
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient

| | |
|---|---|
| **mcvol:** | McGowan's characteristic volume |
| **tf:** | Normal melting (fusion) point |