# Binapacryl

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|---|---|
| **Other names:** | 2-Butenoic acid, 3-methyl-, 2-(1-methylpropyl)-4,6-dinitrophenyl ester |
| | 2-sec-Butyl-4,6-dinitrophenyl 3-methylcrotonate |
| | Crotonic acid, 3-methyl-, 2-sec-butyl-4,6-dinitrophenyl ester |
| | Acricid |
| | Ambox |
| | 2-sek.Butyl-4,6-dinitrofenylester kyseliny 3-methylkrotonove |
| | 2-sec-Butyl-4,6-dinitrophenyl-3,3-dimethylacrylate |
| | 2-sec-Butyl-4,6-dinitrophenyl 3-methyl-2-butenoate |
| | 2-sec-Butyl-4,6-dinitrophenyl senecioate |
| | Dapacryl |
| | 3,3 Dimethyl-acrylate de 2,4-dinitro-6-(1-methylpropyle) phenyle |
| | 3,3-Dimethylacrylic acid 2-sec-butyl-4,6-dinitrophenyl ester |
| | Dinapacryl |
| | 4,6-Dinitro-2-sec-butylphenyl «beta»,«beta»-dimethylacrylate |
| | 2,4-Dinitro-6-sec-butylphenyl 2-methylcrotonate |
| | 4,6-Dinitrophenyl-2-sec-butyl-3-methyl-2-butenonate |
| | Dinoseb, 3,3-dimethylacryl ester |
| | Dinoseb methacrylate |
| | Endosan |
| | ENT 25,793 |
| | FMC 9044 |
| | HOE 2784 |
| | HOE 2784 OA |
| | 3-Methyl-2-butenoic acid 2-sec-butyl-4,6-dinitrophenyl ester |
| | 3-Methyl-2-butenoic acid 2-(1-methylpropyl)-4,6-dinitrophenyl ester |
| | 3-Methylcrotonic acid 2-sec-butyl-4,6-dinitrophenyl ester |
| | (6-(1-Methyl-propyl)-2,4-dinitro-fenyl)-3,3-dimethyl-acrylaat |
| | 2-(1-Methylpropyl)-4,6-dinitrophenyl «beta»,«beta»-dimethacrylate |
| | (6-(1-Methyl-propyl)-2,4-dinitro-phenyl)-3,3-dimethyl-acrylat |
| | (6-(1-Metil-propil)-2,4-dinitro-fenil)-3,3-dimetil-acrilato |
| | Morocide |
| | Morrocid |
| | NIA 9044 |
| | Niagara 9044 |
| | Phenol, 2-sec-butyl-4,6-dinitro-, 3-methylcrotonate |
| | Senecioic acid 2-sec butyl-4,6-dinitrophenyl ester |
| | 2-sec-Butyl-4,6-dinitrophenyl 3-methylcrotonate (binapacryl) |
| **Inchi:** | InChI=1S/C15H18N2O6/c1-5-10(4)12-7-11(16(19)20)8-13(17(21)22)15(12)23-14(18)6-9( |
| **InchiKey:** | ZRDUSMYWDRPZRM-UHFFFAOYSA-N |
| **Formula:** | C15H18N2O6 |

**SMILES:** CCC(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC(=O)C=C(C)C
**Mol. weight [g/mol]:** 322.31
**CAS:** 485-31-4

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 65.35 | kJ/mol | Joback Method |
| hf | -314.98 | kJ/mol | Joback Method |
| hfus | 48.36 | kJ/mol | Joback Method |
| hvap | 95.23 | kJ/mol | Joback Method |
| log10ws | -5.80 | | Crippen Method |
| logp | 3.888 | | Crippen Method |
| mcvol | 236.430 | ml/mol | McGowan Method |
| pc | 1998.33 | kPa | Joback Method |
| rinpol | 2200.00 | | NIST Webbook |
| rinpol | 2247.00 | | NIST Webbook |
| tb | 967.79 | K | Joback Method |
| tc | 1218.59 | K | Joback Method |
| tf | 343.76 ± 0.20 | K | NIST Webbook |
| vc | 0.930 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 726.67 | J/mol×K | 967.79 | Joback Method |
| cpg | 737.63 | J/mol×K | 1009.59 | Joback Method |
| cpg | 747.52 | J/mol×K | 1051.39 | Joback Method |
| cpg | 756.40 | J/mol×K | 1093.19 | Joback Method |
| cpg | 764.33 | J/mol×K | 1134.99 | Joback Method |
| cpg | 771.38 | J/mol×K | 1176.79 | Joback Method |
| cpg | 777.61 | J/mol×K | 1218.59 | Joback Method |
| hfust | 18.89 | kJ/mol | 341.30 | NIST Webbook |

# Sources

| | |
|---|---|
| **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=C485314&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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