# Crotarbital

**Other names:** 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-butenyl)-5-ethyl-
Barbituric acid, 5-(2-butenyl)-5-ethyl-
Barotal
Barotalum
Calypnone
Crotylbarbital
Crotylbarbitalum
Ethyl(crotyl)barbiturate
Go 1046
Kalipnon
Kalypnetten
Kalypnon
Mepertan
5-(2-Butenyl)-5-ethylbarbituric acid
5-Ethyl-5-crotylbarbituric acid
NSC 125735
5-(2-butenyl)-5-ethyl-1H,3H,5H-pyrimidine-2,4,6-trione

**Inchi:** InChI=1S/C10H14N2O3/c1-3-5-6-10(4-2)7(13)11-9(15)12-8(10)14/h3,5H,4,6H2,1-2H3,(H

**InchiKey:** KNMOHCLEINXVBG-HWKANZROSA-N

**Formula:** C10H14N2O3

**SMILES:** CC=CCC1(CC)C(=O)NC(=O)NC1=O

**Mol. weight [g/mol]:** 210.23

**CAS:** 1952-67-6

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -59.85 | kJ/mol | Joback Method |
| hf | -400.43 | kJ/mol | Joback Method |
| hfus | 25.11 | kJ/mol | Joback Method |
| hvap | 63.35 | kJ/mol | Joback Method |
| log10ws | -2.20 | | Crippen Method |
| logp | 0.715 | | Crippen Method |
| mcvol | 161.270 | ml/mol | McGowan Method |
| pc | 3376.28 | kPa | Joback Method |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| tb | 752.71 | K | Joback Method |

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|---|---|---|---|
| tc | 1015.78 | K | Joback Method |
| tf | 643.38 | K | Joback Method |
| vc | 0.602 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 469.85 | J/mol×K | 752.71 | Joback Method |
| cpg | 487.22 | J/mol×K | 796.56 | Joback Method |
| cpg | 503.71 | J/mol×K | 840.40 | Joback Method |
| cpg | 519.37 | J/mol×K | 884.25 | Joback Method |
| cpg | 534.22 | J/mol×K | 928.09 | Joback Method |
| cpg | 548.28 | J/mol×K | 971.94 | Joback Method |
| cpg | 561.60 | J/mol×K | 1015.78 | Joback Method |

# 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=C1952676&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
**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 |