# CROTETHAMIDE

**Other names:** 2-Butenamide, N-[1-[(dimethylamino)carbonyl]propyl]-N-ethyl-
Crotethamide
N-[1-(Dimethylcarbamoyl)propyl]-N-ethylcrotonamide
Crotethamid
**Inchi:** InChI=1S/C12H22N2O2/c1-6-9-11(15)14(8-3)10(7-2)12(16)13(4)5/h6,9-10H,7-8H2,1-5H3
**InchiKey:** LSAMUAYPDHUBQD-TWGQIWQCSA-N
**Formula:** C12H22N2O2
**SMILES:** C/C=C/C(=O)N(CC)C(CC)C(=O)N(C)C
**Mol. weight [g/mol]:** 226.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 32.75 | kJ/mol | Joback Method |
| ie | 8.01 | eV | Cheméo Relay (1.0) |
| logp | 1.278 | | Crippen Method |
| mcvol | 198.740 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 517.27 | J/mol×K | 610.30 | Joback Method |
| cpg | 532.90 | J/mol×K | 641.12 | Joback Method |
| cpg | 547.66 | J/mol×K | 671.95 | Joback Method |
| cpg | 561.61 | J/mol×K | 702.77 | Joback Method |
| cpg | 574.79 | J/mol×K | 733.60 | Joback Method |
| cpg | 587.23 | J/mol×K | 764.42 | Joback Method |
| cpg | 598.98 | J/mol×K | 795.25 | Joback Method |

## Sources

**Cheméo Relay (1.0, beta):**

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6168769&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 |
| **Cheméo Relay (1.0):** | |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **ie:** | Ionization energy |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |