

# 1,6-Cleve's acid

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 5-Amino-2-naphthalenesulfonic acid<br>1-Aminonaphthalene-6-sulfonic acid<br>2-Naphthalenesulfonic acid, 5-amino-<br>Cleve's «beta»-acid<br>Cleve's acid-1,6<br>Kyselina cleve<br>Kyselina 1-naftylamin-6-sulfonova<br>1-Amino-6-naphthalenesulfonic acid<br>1-Amino-6-sulfonaphthalene<br>1-Naphthylamine-6-sulfonic acid<br>5-Naphthylamine-2-sulfonic acid<br>«alpha»-Naphthylamine-6-sulfonic acid<br>NSC 31506<br>5-aminonaphthalene-2-sulphonic acid |
| Inchi:               | InChI=1S/C10H9NO3S/c11-10-3-1-2-7-6-8(15(12,13)14)4-5-9(7)10/h1-6H,11H2,(H,12,13)                                                                                                                                                                                                                                                                                                                                                                         |
| InchiKey:            | UWPJYQYRSWYIGZ-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Formula:             | C10H9NO3S                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| SMILES:              | Nc1cccc2cc(S(=O)(=O)O)ccc12                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Mol. weight [g/mol]: | 223.25                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| CAS:                 | 119-79-9                                                                                                                                                                                                                                                                                                                                                                                                                                                  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -305.79 | kJ/mol  | Joback Method  |
| hf            | -416.86 | kJ/mol  | Joback Method  |
| hfus          | 32.60   | kJ/mol  | Joback Method  |
| hvap          | 89.05   | kJ/mol  | Joback Method  |
| log10ws       | -2.50   |         | Crippen Method |
| logp          | 1.669   |         | Crippen Method |
| mcvol         | 152.480 | ml/mol  | McGowan Method |
| pc            | 5670.27 | kPa     | Joback Method  |
| tb            | 696.31  | K       | Joback Method  |
| tc            | 915.54  | K       | Joback Method  |
| tf            | 469.26  | K       | Joback Method  |
| vc            | 0.584   | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 384.65 | J/mol×K | 696.31          | Joback Method |
| cpg           | 394.35 | J/mol×K | 732.85          | Joback Method |
| cpg           | 403.26 | J/mol×K | 769.39          | Joback Method |
| cpg           | 411.43 | J/mol×K | 805.93          | Joback Method |
| cpg           | 418.88 | J/mol×K | 842.47          | Joback Method |
| cpg           | 425.66 | J/mol×K | 879.00          | Joback Method |
| cpg           | 431.79 | J/mol×K | 915.54          | Joback Method |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C119799&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C119799&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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