

# 2-HYDROXY-3-PHENYLBENZOIC ACID

|                      |                                                                                                                                                                                                                                     |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 3-Phenylsalicylic acid<br>[1,1'-Biphenyl]-3-carboxylic acid, 2-hydroxy-<br>m-Phenylsalicylic acid<br>Salicylic acid, 3-phenyl-<br>USAF do-59<br>3-Biphenylcarboxylic acid, 2-hydroxy-<br>2-Hydroxy[1,1'-biphenyl]-3-carboxylic acid |
| Inchi:               | InChI=1S/C13H10O3/c14-12-10(9-5-2-1-3-6-9)7-4-8-11(12)13(15)16/h1-8,14H,(H,15,16)                                                                                                                                                   |
| InchiKey:            | ZJWUEJOPKFYFQD-UHFFFAOYSA-N                                                                                                                                                                                                         |
| Formula:             | C13H10O3                                                                                                                                                                                                                            |
| SMILES:              | O=C(O)c1cccc(-c2ccccc2)c1O                                                                                                                                                                                                          |
| Mol. weight [g/mol]: | 214.22                                                                                                                                                                                                                              |

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.8313  |         | Cheméo Relay (1.0) |
| hf            | -378.51 | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 28.59   | kJ/mol  | Joback Method      |
| hvap          | 118.35  | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 8.03    | eV      | Cheméo Relay (1.0) |
| log10ws       | -3.13   |         | Cheméo Relay (1.0) |
| logp          | 2.757   |         | Crippen Method     |
| mcvol         | 159.820 | ml/mol  | McGowan Method     |
| pc            | 4356.87 | kPa     | Joback Method      |
| tb            | 606.47  | K       | Cheméo Relay (1.0) |
| tc            | 942.23  | K       | Cheméo Relay (1.0) |
| tf            | 442.83  | K       | Cheméo Relay (1.0) |
| vc            | 0.564   | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 431.77 | J/mol×K | 781.85          | Joback Method |
| cpg           | 441.64 | J/mol×K | 821.48          | Joback Method |

|       |           |         |         |               |
|-------|-----------|---------|---------|---------------|
| cpg   | 450.90    | J/mol×K | 861.10  | Joback Method |
| cpg   | 459.64    | J/mol×K | 900.73  | Joback Method |
| cpg   | 467.98    | J/mol×K | 940.36  | Joback Method |
| cpg   | 476.03    | J/mol×K | 979.99  | Joback Method |
| cpg   | 483.92    | J/mol×K | 1019.61 | Joback Method |
| dvisc | 0.0001208 | Pa×s    | 524.10  | Joback Method |
| dvisc | 0.0000506 | Pa×s    | 567.06  | Joback Method |
| dvisc | 0.0000239 | Pa×s    | 610.02  | Joback Method |
| dvisc | 0.0000125 | Pa×s    | 652.98  | Joback Method |
| dvisc | 0.0000071 | Pa×s    | 695.93  | Joback Method |
| dvisc | 0.0000043 | Pa×s    | 738.89  | Joback Method |
| dvisc | 0.0000027 | Pa×s    | 781.85  | Joback Method |

## Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C304063&Units=SI>

Joback Method: [https://en.wikipedia.org/wiki/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](https://www.chemeo.com/doc/models/crippen_log10ws)

Cheméo Relay (1.0):

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>ie:</b>      | Ionization energy                               |
| <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                            |

**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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