N-Phenylmaleamic acid

Other names: 2-Butenoic acid, 4-oxo-4-(phenylamino)-, (Z)-; 4-Oxo-4-phenylamino-2-butenoic acid; 4-oxo-4-(phenylamino)isocrotonic acid; Maleamic acid, N-phenyl-; Maleanilic acid; Maleanilinic acid; Maleic acid monoanilide.

InChI: InChI=1S/C10H9NO3/c12-9(6-7-10(13)14)11-8-4-2-1-3-5-8/h1-7H,(H,11,12)(H,13,14)/b7-6-

InChI Key: WHZLCOICKHPRL-SREVYHEPSA-N

Formula: C10H9NO3

SMILES: O=C(O)C=CC(O)=Nc1ccccc1

Molecular Weight: 191.18

CAS: 555-59-9

Physical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta_{f}H^\circ_{gas}$</td>
<td>-240.59</td>
<td>kJ/mol</td>
<td>Joback Method</td>
</tr>
<tr>
<td>$\Delta_{vap}H^\circ$</td>
<td>83.59</td>
<td>kJ/mol</td>
<td>Joback Method</td>
</tr>
<tr>
<td>$logP_{oct/wat}$</td>
<td>1.92</td>
<td></td>
<td>Crippen Method</td>
</tr>
<tr>
<td>$P_c$</td>
<td>3682.02</td>
<td>kPa</td>
<td>Joback Method</td>
</tr>
<tr>
<td>$T_{boil}$</td>
<td>773.83</td>
<td>K</td>
<td>Joback Method</td>
</tr>
<tr>
<td>$T_c$</td>
<td>985.62</td>
<td>K</td>
<td>Joback Method</td>
</tr>
</tbody>
</table>

Sources


NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H9NO3/c12-9(6-7-10(13)14)11-8-4-2-1-3-5-8/h1-7H,(H,11,12)(H,13,14)/b7-6-

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_{f}H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{vap}H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient.

$P_c$: Critical Pressure (kPa).
$T_{\text{boil}}$: Normal Boiling Point Temperature (K).
$T_c$: Critical Temperature (K).

Latest version available from:
https://www.chemeo.com/cid/91-820-0/N-Phenylmaleamic%20acid
Generated by Cheméo on Wed, 14 Aug 2019 02:29:04 +0000.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.