

Imidodicarbonimidic diamide, N-(2-phenylethyl)-

Other names:

1-phenethylbiguanide
Biguanide, 1-phenethyl-
Cronoformin
DB Comb
DB-retard
DBI
Diabis
Dibiraf
Dibotin
Fenfoduron
Fenformin
Fenformina
Fenormin
Glukopostin
Glyphen
N'-«beta»-Fenetilformamidiniliminourea
N'-«beta»-Phenethylformamidinyliminourea
N-(2-phenylethyl)imidodicarbonimidic diamide
NCI-C01741
PEDG
Phenethyldiguanide
Phenformin
Phenformine
Phenformix
Phenylethylbiguanide
Retardo
W 32
debeone
«beta»-PEBG
«beta»-Phenethylbiguanide

Inchi: InChI=1S/C10H15N5/c11-9(12)15-10(13)14-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2,(H6,11,12,13)

InchiKey: ICFJFFQQQTFMIBG-UHFFFAOYSA-N

Formula: C10H15N5

SMILES: N=C(N)NC(=N)NCCc1ccccc1

Mol. weight [g/mol]: 205.26

CAS: 114-86-3

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--|
| gf | 798.16 | kJ/mol | Joback Method |
| hf | 524.19 | kJ/mol | Joback Method |
| hvap | 87.80 | kJ/mol | Joback Method |
| log10ws | -4.74 | | Crippen Method |
| logp | 0.237 | | Crippen Method |
| mcvol | 169.300 | ml/mol | McGowan Method |
| tb | 796.43 | K | Joback Method |
| tf | 555.02 | K | Joback Method |
| tt | 446.85 | K | Thermodynamic Solubility and Mixing Properties of Phenformin in 14 Pure Solvents at Temperatures Ranging from 278.15 to 323.15 K |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 495.40 | J/mol×K | 796.43 | Joback Method |
| cpg | 42.66 | J/mol×K | 100.12 | Joback Method |
| cpg | 42.66 | J/mol×K | 100.12 | Joback Method |
| cpg | 42.66 | J/mol×K | 100.12 | Joback Method |
| cpg | 42.66 | J/mol×K | 100.12 | Joback Method |
| cpg | 42.66 | J/mol×K | 100.12 | Joback Method |
| cpg | 42.66 | J/mol×K | 100.12 | Joback Method |
| cpg | 42.66 | J/mol×K | 100.12 | Joback Method |

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Thermodynamic Solubility and Mixing Properties of Phenformin in 14 Pure Solvents at Temperatures Ranging from 278.15 to 323.15 K:
Joback Method:
McGowan Method:

<https://www.doi.org/10.1021/acs.jced.9b00844>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C114863&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 |
| 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 |
| tb: | Normal Boiling Point Temperature |
| tf: | Normal melting (fusion) point |
| tt: | Triple Point Temperature |

Latest version available from:

<https://www.chemeo.com/cid/85-715-4/Imidodicarbonimidic-diamide-N-2-phenylethyl.pdf>

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