

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:

ICFJFFQQTFMIBG-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

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan 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
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:	https://www.doi.org/10.1021/acs.jced.9b00844

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

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