2,4-Diamino-6-phenyl-s-triazine

Other names:	s-Triazine, 2,4-diamino-6-phenyl-
	Benzoguanamine
	Benzoguanimine
	ENT 60118
	2,4-Diamino-6-phenyl-s-triazine
	2,4-Diamino-6-phenyl-1,3,5-triazine
	2,6-Diamino-4-phenyl-1,3,5-triazine
	6-Phenyl-1,3,5-triazine-2,4-diamine
	USAF RH-5
	2-Phenyl-4,6-diamino-s-triazine
	2-Phenyl-4,6-diamino-1,3,5-triazine
	4,6-Diamino-2-phenyl-s-triazine
	NSC 3267
	6-phenyl-1,3,5-triazine-2,4-diyldiamine
Inchi:	InChI=1S/C9H9N5/c10-8-12-7(13-9(11)14-8)6-4-2-1-3-5-6/h1-5H,(H4,10,11,12,13,14)
InchiKey:	GZVHEAJQGPRDLQ-UHFFFAOYSA-N
Formula:	C9H9N5
SMILES:	Nc1nc(N)nc(-c2ccccc2)n1
Mol. weight [g/mol]:	187.21

Physical Properties

Property code	Value	Unit	Source
af	0.6327		Cheméo Relay (1.0)
gf	469.88	kJ/mol	Cheméo Relay (1.0, beta)
hf	199.75	kJ/mol	Cheméo Relay (1.0)
hvap	118.74	kJ/mol	Cheméo Relay (1.0)
ie	8.72	eV	Cheméo Relay (1.0)
log10ws	-3.47		Cheméo Relay (1.0)
logp	0.703		Crippen Method
mcvol	140.050	ml/mol	McGowan Method
pc	4883.89	kPa	Cheméo Relay (1.0, beta)
tb	593.12	K	Cheméo Relay (1.0)
tc	945.76	K	Cheméo Relay (1.0)
tf	480.75	K	Cheméo Relay (1.0)
vc	0.520	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91769&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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