

Guanidine, 2-benzyl-1,3-dimethyl-

Other names:	2-Benzyl-1,3-dimethylguanidine Guanidine, N,N'-dimethyl-N''-(phenylmethyl)- Bethanidine 1-Benzyl-2,3-dimethylguanidine
Inchi:	InChI=1S/C10H15N3/c1-11-10(12-2)13-8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3,(H2,11,12,13)
InchiKey:	NIVZHWNOUVJHKV-UHFFFAOYSA-N
Formula:	C10H15N3
SMILES:	CN=C(NC)NCc1ccccc1
Mol. weight [g/mol]:	177.25
CAS:	55-73-2

Physical Properties

Property code	Value	Unit	Source
hf	166.17	kJ/mol	Joback Method
hvap	56.40	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	0.981		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	631.78	K	Joback Method
tc	858.16	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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