1-Phenyl-3-o-tolylguanidine

Inchi: InChI=1S/C14H15N3/c1-11-7-5-6-10-13(11)17-14(15)16-12-8-3-2-4-9-12/h2-10H,1H3,(H
InchiKey: IKOWCCQMFQLCGP-UHFFFAOYSA-N
Formula: C14H15N3
SMILES: Cc1ccccc1NC(=N)Nc1ccccc1
Mol. weight [g/mol]: 225.29
CAS: 6268-14-0

Physical Properties

Property code	Value	Unit	Source
gf	664.57	kJ/mol	Joback Method
hf	434.57	kJ/mol	Joback Method
hvap	76.92	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.454		Crippen Method
mcvol	186.240	ml/mol	McGowan Method
tb	762.74	K	Joback Method
tf	487.00	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.60	J/mol×K	762.74	Joback Method
cpg	41.37	J/mol×K	100.12	Joback Method
cpg	41.37	J/mol×K	100.12	Joback Method
cpg	41.37	J/mol×K	100.12	Joback Method
cpg	41.37	J/mol×K	100.12	Joback Method
cpg	41.37	J/mol×K	100.12	Joback Method
cpg	41.37	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=C6268140&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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