

3,3'-Diaminobenzophenone

Other names:	Methanone, bis(3-aminophenyl)-
Inchi:	InChI=1S/C13H12N2O/c14-11-5-1-3-9(7-11)13(16)10-4-2-6-12(15)8-10/h1-8H,14-15H2
InchiKey:	TUQQUUXMCKXGDI-UHFFFAOYSA-N
Formula:	C13H12N2O
SMILES:	<chem>Nc1cccc(C(=O)c2cccc(N)c2)c1</chem>
Mol. weight [g/mol]:	212.25
CAS:	611-79-0

Physical Properties

Property code	Value	Unit	Source
gf	268.12	kJ/mol	Joback Method
hf	93.47	kJ/mol	Joback Method
hfus	28.72	kJ/mol	Joback Method
hvap	78.44	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.082		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	759.09	K	Joback Method
tc	1022.73	K	Joback Method
tf	530.60	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.40	J/molxK	759.09	Joback Method
cpg	464.90	J/molxK	803.03	Joback Method
cpg	476.24	J/molxK	846.97	Joback Method
cpg	486.50	J/molxK	890.91	Joback Method
cpg	495.77	J/molxK	934.85	Joback Method
cpg	504.11	J/molxK	978.79	Joback Method
cpg	511.62	J/molxK	1022.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=C611790&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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