2,5-Diaminobenzophenone

Other names: (2,5-Diaminophenyl)(phenyl)methanone
Benzophenone, 2,5-diamino
Methanone, (2,5-diaminophenyl)phenyl-
Inchi: InChI=1S/C13H12N2O/c14-10-6-7-12(15)11(8-10)13(16)9-4-2-1-3-5-9/h1-8H,14-15H2
InchiKey: WJWKTVHKQDEXEQ-UHFFFAOYSA-N
Formula: C13H12N2O
SMILES: Nc1ccc(N)c(C(=O)c2ccccc2)c1
Mol. weight [g/mol]: 212.25
CAS: 18330-94-4

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
rinpol	2198.00		NIST Webbook
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/mol×K	759.09	Joback Method
cpg	464.90	J/mol×K	803.03	Joback Method
cpg	476.24	J/mol×K	846.97	Joback Method
cpg	486.50	J/mol×K	890.91	Joback Method
cpg	495.77	J/mol×K	934.85	Joback Method

cpg	504.11	J/mol×K	978.79	Joback Method
cpg	511.62	J/mol×K	1022.73	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=C18330944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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