1,3-Bis(anilino)propane

Other names: N,N'-diphenylpropane-1,3-diamine
Inchi: InChI=1S/C15H18N2/c1-3-8-14(9-4-1)16-12-7-13-17-15-10-5-2-6-11-15/h1-6,8-11,16-17
InchiKey: JQMRSZJEVQNIPB-UHFFFAOYSA-N
Formula: C15H18N2
SMILES: c1ccc(NCCCNc2ccccc2)cc1
Mol. weight [g/mol]: 226.32
CAS: 104-69-8

Physical Properties

Property code	Value	Unit	Source
gf	479.02	kJ/mol	Joback Method
hf	227.07	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	66.41	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.601		Crippen Method
mcvol	194.650	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
tb	696.30	K	Joback Method
tc	926.96	K	Joback Method
tf	416.97	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.46	J/mol×K	696.30	Joback Method
cpg	545.95	J/mol×K	734.74	Joback Method
cpg	561.18	J/mol×K	773.19	Joback Method
cpg	575.25	J/mol×K	811.63	Joback Method
cpg	588.22	J/mol×K	850.07	Joback Method
cpg	600.18	J/mol×K	888.51	Joback Method
cpg	611.22	J/mol×K	926.96	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=C104698&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
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