

Aniline, p,p'-(p-phenylenedioxy)di-

Other names:	1,4-Phenylene-di-4-aminophenyl ether Benzenamine,4,4'-[1,4-phenylenebis(oxy)]bis-
Inchi:	InChI=1S/C18H16N2O2/c19-13-1-5-15(6-2-13)21-17-9-11-18(12-10-17)22-16-7-3-14(20)
InchiKey:	JCRRFJIVUPSNTA-UHFFFAOYSA-N
Formula:	C18H16N2O2
SMILES:	<chem>Nc1ccc(Oc2ccc(Oc3ccc(N)cc3)cc2)cc1</chem>
Mol. weight [g/mol]:	292.33
CAS:	3491-12-1

Physical Properties

Property code	Value	Unit	Source
gf	331.92	kJ/mol	Joback Method
hf	63.47	kJ/mol	Joback Method
hfus	36.10	kJ/mol	Joback Method
hvap	90.58	kJ/mol	Joback Method
ie	6.60	eV	NIST Webbook
log10ws	-4.01		Crippen Method
logp	4.436		Crippen Method
mcvol	224.900	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	896.12	K	Joback Method
tc	1163.63	K	Joback Method
tf	620.42	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.10	J/molxK	896.12	Joback Method
cpg	677.74	J/molxK	940.71	Joback Method
cpg	688.86	J/molxK	985.29	Joback Method
cpg	698.53	J/molxK	1029.88	Joback Method
cpg	706.80	J/molxK	1074.46	Joback Method
cpg	713.75	J/molxK	1119.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3491121&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
ie:	Ionization energy
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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