

Benzenamine, 4-phenoxy-

Other names:	Aniline, p-phenoxy- p-Aminophenyl phenyl ether p-Phenoxyaniline 4-Amino-1-phenoxybenzene 4-Aminodiphenyl ether 4-Aminophenyl phenyl ether 4-Phenoxyaniline 4-Phenoxaniline Ether, 4-aminophenyl phenyl 4-Aminodifenylether 4-Aminobiphenyl ether 4-(Phenyloxy)aniline 4-Phenoxybenzenamine NSC 4629
Inchi:	InChI=1S/C12H11NO/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9H,13H2
InchiKey:	WOYZXEUVWXQVNV-UHFFFAOYSA-N
Formula:	C12H11NO
SMILES:	<chem>Nc1ccc(Oc2ccccc2)cc1</chem>
Mol. weight [g/mol]:	185.22
CAS:	139-59-3

Physical Properties

Property code	Value	Unit	Source
gf	226.80	kJ/mol	Joback Method
hf	72.15	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	60.57	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	3.061		Crippen Method
mcvol	148.270	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	627.25	K	Joback Method
tc	881.74	K	Joback Method
tf	356.50 ± 0.50	K	NIST Webbook
vc	0.538	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.85	J/mol×K	627.25	Joback Method
cpg	374.56	J/mol×K	669.67	Joback Method
cpg	388.09	J/mol×K	712.08	Joback Method
cpg	400.50	J/mol×K	754.50	Joback Method
cpg	411.83	J/mol×K	796.91	Joback Method
cpg	422.13	J/mol×K	839.33	Joback Method
cpg	431.47	J/mol×K	881.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	461.20	K	1.90	NIST Webbook
tbrp	461.00 ± 1.00	K	1.90	NIST Webbook

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=C139593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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