

Phenol, 4-(phenylamino)-

Other names:	p-Anilinophenol 4-Anilinophenol p-Hydroxydiphenylamine 4-Hydroxydiphenylamine p-Oxydiphenylamine Phenol, p-anilino- N-Phenyl-p-aminophenol p-(Phenylamino)phenol VTI 1 p-Hydroxydifenylamin Diphenylamine, 4-hydroxy- Phenyl-p-aminophenol para-Hydroxydifenylamin 4-Phenylaminophenol NSC 1543
Inchi:	InChI=1S/C12H11NO/c14-12-8-6-11(7-9-12)13-10-4-2-1-3-5-10/h1-9,13-14H
InchiKey:	JTTMYKSFKOOQLP-UHFFFAOYSA-N
Formula:	C12H11NO
SMILES:	Oc1ccc(Nc2ccccc2)cc1
Mol. weight [g/mol]:	185.22
CAS:	122-37-2

Physical Properties

Property code	Value	Unit	Source
gf	209.75	kJ/mol	Joback Method
hf	58.21	kJ/mol	Joback Method
hfus	25.80	kJ/mol	Joback Method
hvap	66.31	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	3.136		Crippen Method
mcvol	148.270	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	658.11	K	Joback Method
tc	914.96	K	Joback Method
tf	442.22	K	Joback Method
vc	0.492	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.27	J/mol×K	658.11	Joback Method
cpg	389.75	J/mol×K	700.92	Joback Method
cpg	402.08	J/mol×K	743.73	Joback Method
cpg	413.43	J/mol×K	786.54	Joback Method
cpg	423.95	J/mol×K	829.35	Joback Method
cpg	433.80	J/mol×K	872.15	Joback Method
cpg	443.12	J/mol×K	914.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	488.70	K	1.60	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=C122372&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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