

Phenol, 4-[(phenylmethyl)amino]-

Other names:	Phenol, p-(benzylamino)- p-(Benzylamino)phenol N-Benzyl-p-aminophenol 4-(Benzylamino)phenol 4-(N-Benzylamino)phenol 4-[(Phenylmethyl)amino]phenol N-(4-Hydroxyphenyl)benzylamine
Inchi:	InChI=1S/C13H13NO/c15-13-8-6-12(7-9-13)14-10-11-4-2-1-3-5-11/h1-9,14-15H,10H2
InchiKey:	SRYYOKKLTBRLHT-UHFFFAOYSA-N
Formula:	C13H13NO
SMILES:	Oc1ccc(NCc2ccccc2)cc1
Mol. weight [g/mol]:	199.25
CAS:	103-14-0

Physical Properties

Property code	Value	Unit	Source
gf	218.17	kJ/mol	Joback Method
hf	37.57	kJ/mol	Joback Method
hfus	28.39	kJ/mol	Joback Method
hvap	68.53	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.004		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
tb	680.99	K	Joback Method
tc	931.94	K	Joback Method
tf	453.49	K	Joback Method
vc	0.548	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.94	J/mol×K	680.99	Joback Method
cpg	440.02	J/mol×K	722.82	Joback Method

cpg	452.99	J/mol×K	764.64	Joback Method
cpg	464.99	J/mol×K	806.47	Joback Method
cpg	476.18	J/mol×K	848.29	Joback Method
cpg	486.70	J/mol×K	890.12	Joback Method
cpg	496.71	J/mol×K	931.94	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=C103140&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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