

4-Amino-3-phenyl phenol

Inchi:	InChI=1S/C12H11NO/c13-12-7-6-10(14)8-11(12)9-4-2-1-3-5-9/h1-8,14H,13H2
InchiKey:	ACTPUQAHTZXJSC-UHFFFAOYSA-N
Formula:	C12H11NO
SMILES:	Nc1ccc(O)cc1-c1ccccc1
Mol. weight [g/mol]:	185.22
CAS:	103114-32-5

Physical Properties

Property code	Value	Unit	Source
gf	177.18	kJ/mol	Joback Method
hf	27.06	kJ/mol	Joback Method
hfus	25.51	kJ/mol	Joback Method
hvap	71.17	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.641		Crippen Method
mcvol	148.270	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
tb	685.45	K	Joback Method
tc	952.23	K	Joback Method
tf	485.34	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.51	J/molxK	685.45	Joback Method
cpg	395.35	J/molxK	729.91	Joback Method
cpg	407.14	J/molxK	774.38	Joback Method
cpg	418.05	J/molxK	818.84	Joback Method
cpg	428.24	J/molxK	863.30	Joback Method
cpg	437.86	J/molxK	907.77	Joback Method
cpg	447.08	J/molxK	952.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103114325&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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