3-Hydroxydiphenylamine

Other names: m-Hydroxydiphenylamine
Phenol, 3-(phenylamino)-
m-Anilinophenol
Phenol, m-anilino-
3-(Phenylamino)phenol
3-Hydroxy-N-phenylaniline
Inchi: InChI=1S/C12H11NO/c14-12-8-4-7-11(9-12)13-10-5-2-1-3-6-10/h1-9,13-14H
InchiKey: NDACNGSDAFKTGE-UHFFFAOYSA-N
Formula: C12H11NO
SMILES: Oc1cccc(Nc2ccccc2)c1
Mol. weight [g/mol]: 185.22
CAS: 101-18-8

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	613.20	K	NIST Webbook
tc	914.96	K	Joback Method
tf	442.22	K	Joback Method
vc	0.492	m3/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

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101188&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
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