

3-HYDROXYDIPHENYLAMINE

Other names:	3-(Phenylamino)phenol 3-Hydroxy-N-phenylaniline Phenol, 3-(phenylamino)- Phenol, m-anilino- m-Anilinophenol m-Hydroxydiphenylamine
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]:	185.23

Physical Properties

Property code	Value	Unit	Source
af	0.6381		Cheméo Relay (1.0)
gf	209.75	kJ/mol	Joback Method
hf	22.45	kJ/mol	Cheméo Relay (1.0)
hfus	25.80	kJ/mol	Joback Method
hvap	99.83	kJ/mol	Cheméo Relay (1.0)
ie	7.35	eV	Cheméo Relay (1.0)
log10ws	-2.96		Cheméo Relay (1.0)
logp	3.136		Crippen Method
mcvol	148.270	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	623.18	K	Cheméo Relay (1.0)
tc	940.44	K	Cheméo Relay (1.0)
tf	380.84	K	Cheméo Relay (1.0)
vc	0.519	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101188&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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