N-Phenylbenzohydroxamic acid

Other names:	N-Benzoyl-N-phenylhydroxamic acid
	N-Benzoylphenylhydroxylamine
	N-Phenylbenzohyroxamic acid
	N-benzoyl-N-phenylhydroxylamine
	N-hydroxy-N-phenylbenzamide
	N-hydroxybenzanilide
	NSC 42454
	benzamide, N-hydroxy-N-phenyl-
	benzohydroxamic acid, N-phenyl-
Inchi:	InChI=1S/C13H11NO2/c15-13(11-7-3-1-4-8-11)14(16)12-9-5-2-6-10-12/h1-10,16H
InchiKey:	YLYIXDZITBMCIW-UHFFFAOYSA-N
Formula:	C13H11NO2
SMILES:	O=C(c1ccccc1)N(O)c1ccccc1
Mol. weight [g/mol]:	213.24

Physical Properties

Property code	Value	Unit	Source
af	0.7466		Cheméo Relay (1.0)
gf	128.44	kJ/mol	Joback Method
hf	-32.48	kJ/mol	Cheméo Relay (1.0)
hfus	26.22	kJ/mol	Joback Method
hvap	96.11	kJ/mol	Cheméo Relay (1.0)
ie	8.50	eV	Cheméo Relay (1.0)
log10ws	-1.89		Aqueous Solubility Prediction Method
logp	2.723		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	610.09	K	Cheméo Relay (1.0)
tc	920.53	K	Cheméo Relay (1.0)
tf	394.15	K	Volumetric and steric properties of hydroxamic acids in ethanol at different temperatures
tf	394.15	K	Steric parameters and excess properties of hydroxamic acids

tf	394.15	K	Partial Molar Volumes and Viscosity B-Coefficient of N-Phenylbenzohydroxamic Acid in Dimethylsulfoxide at Different Temperatures
vc	0.606	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.18	J/mol×K	708.69	Joback Method
cpg	441.05	J/mol×K	746.44	Joback Method
cpg	451.92	J/mol×K	784.19	Joback Method
cpg	461.87	J/mol×K	821.94	Joback Method
cpg	470.98	J/mol×K	859.69	Joback Method
cpg	479.32	J/mol×K	897.44	Joback Method
cpg	486.96	J/mol×K	935.19	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0, beta):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0):	
Volumetric and steric properties of hydroxamic acids in ethanol at different temperatures:	https://www.doi.org/10.1016/j.jct.2012.03.019
Steric parameters and excess properties of hydroxamic acids:	https://www.doi.org/10.1016/j.jct.2012.03.020
Partial Molar Volumes and Viscosity B-Coefficient of N-Phenylbenzohydroxamic Acid in Dimethylsulfoxide at Different Temperatures:	https://www.doi.org/10.1021/je7006956
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C304881&Units=SI

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