2,2'-Bipyridine

Other names:	.alpha.,.alpha.'-bipyridyl
	.alpha.,.alpha.'-dipyridine
	2,2'-Bipyridin
	2,2'-Bipyridyl
	2,2'-Dipyridine
	2,2'-Dipyridyl
	2,2´-bipyridine
	2-(2-Pyridyl)pyridine
	AA-DP
	Bipyridine
	CI 588
	NSC 1550
	NSC 615009
	«alpha»,«alpha»'-Bipyridine
	«alpha»,«alpha»'-Bipyridyl
	«alpha»,«alpha»'-Dipyridine
	«alpha»,«alpha»'-Dipyridyl
	Â«alphaÂ»,Â«alphaÂ»'-Bipyridine
	Â«alphaÂ»,Â«alphaÂ»'-Bipyridyl
	Â«alphaÂ»,Â«alphaÂ»'-Dipyridine
	Â«alphaÂ»,Â«alphaÂ»'-Dipyridyl
Inchi:	InChI=1S/C10H8N2/c1-3-7-11-9(5-1)10-6-2-4-8-12-10/h1-8H
InchiKey:	ROFVEXUMMXZLPA-UHFFFAOYSA-N
Formula:	C10H8N2
SMILES:	c1ccc(-c2ccccn2)nc1
Mol. weight [g/mol]:	156.18
CAS:	366-18-7

Physical Properties

Property code	Value	Unit	Source
basg	933.40 ± 6.30	kJ/mol	NIST Webbook
basg	908.00	kJ/mol	NIST Webbook
chs	-5285.50 ± 4.70	kJ/mol	NIST Webbook
chs	-5264.50 ± 1.50	kJ/mol	NIST Webbook
hf	289.00 ± 5.20	kJ/mol	NIST Webbook
hf	267.90 ± 3.00	kJ/mol	NIST Webbook

hfs	186.10 ± 2.00	kJ/mol	NIST Webbook
hfs	207.10 ± 4.90	kJ/mol	NIST Webbook
hsub	81.80 ± 2.30	kJ/mol	NIST Webbook
hsub	81.80	kJ/mol	NIST Webbook
hsub	81.80 ± 2.30	kJ/mol	NIST Webbook
hsub	75.00 ± 5.00	kJ/mol	NIST Webbook
hsub	81.90	kJ/mol	NIST Webbook
hvap	67.00 ± 2.30	kJ/mol	NIST Webbook
ie	8.35 ± 0.02	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
log10ws	-1.42		Aqueous Solubility Prediction Method
logp	2.144		Crippen Method
mcvol	124.200	ml/mol	McGowan Method
rinpol	245.48		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	245.68		NIST Webbook
rinpol	247.15		NIST Webbook
rinpol	1444.00		NIST Webbook
ripol	2193.00		NIST Webbook
tb	545.60	K	NIST Webbook
tb	546.70	K	NIST Webbook
tf	342.60	K	NIST Webbook
tt	343.05 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.40	kJ/mol	345.00	NIST Webbook
hvapt	67.00	kJ/mol	298.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds

Sources

Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds:	https://www.doi.org/10.1021/je900034d
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C366187&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of 2,2'-Bipyridine and 4,4'-Dimethyl-2,2'-bipyridine in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je700269m

Legend

basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

Latest version available from:
https://www.chemeo.com/cid/55-757-1/2-2-Bipyridine.pdf
Generated by Cheméo on 2024-04-28 16:53:21.860424753 +0000 UTC m=+16612450.781002068.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.