

4,4'-Bipyridine

Other names:	.gamma.,.gamma.'-bipyridyl .gamma.,.gamma.'-dipyridyl 4,4'-Bipyridyl 4,4'-Dipyridine 4,4'-Dipyridyl 4,4-Bipyridine 4,4-Bipyridyl 4,4-Dipyridyl 4,4'-bipyridine 4-(4-Pyridyl)pyridine Bipyridine, 4,4'- NSC 404423 «gamma», «gamma»'-Bipyridyl «gamma», «gamma»'-Dipyridyl Â«gammaÂ», Â«gammaÂ»'-Bipyridyl Â«gammaÂ», Â«gammaÂ»'-Dipyridyl
Inchi:	InChI=1S/C10H8N2/c1-5-11-6-2-9(1)10-3-7-12-8-4-10/h1-8H
InchiKey:	MWVTWFVJZLCBMC-UHFFFAOYSA-N
Formula:	C10H8N2
SMILES:	c1cc(-c2ccncc2)ccn1
Mol. weight [g/mol]:	156.18
CAS:	553-26-4

Physical Properties

Property code	Value	Unit	Source
basg	900.00 ± 10.00	kJ/mol	NIST Webbook
chs	-5265.20 ± 1.80	kJ/mol	NIST Webbook
hf	293.10 ± 3.60	kJ/mol	NIST Webbook
hfs	186.80 ± 2.20	kJ/mol	NIST Webbook
hfus	16.10	kJ/mol	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds
hsub	106.30	kJ/mol	NIST Webbook
hsub	106.30 ± 2.80	kJ/mol	NIST Webbook
hsub	106.30 ± 2.80	kJ/mol	NIST Webbook

hvap	71.10 ± 2.60	kJ/mol	NIST Webbook
ie	9.10 ± 0.02	eV	NIST Webbook
log10ws	-1.54		Aqueous Solubility Prediction Method
logp	2.144		Crippen Method
mcvol	124.200	ml/mol	McGowan Method
rinpol	1507.00		NIST Webbook
rinpol	1507.00		NIST Webbook
ripol	2453.00		NIST Webbook
tb	578.00	K	NIST Webbook
tb	578.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	16.10	kJ/mol	377.50	NIST Webbook

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: Crippen Method.

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C553264&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
hfus:	Enthalpy of fusion 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
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

Latest version available from:

<https://www.cheméo.com/cid/20-286-2/4-4-Bipyridine.pdf>

Generated by Cheméo on 2024-04-29 04:53:49.921302639 +0000 UTC m=+16655678.841879954.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.