BIS(3-PYRIDYLMETHYL)AMINE

Other names: 3-Pyridinemethanamine, N-(3-pyridinylmethyl)-
Bis((3-pyridyl)methyl)amine
Pyridine, 3,3'-(iminodimethylene)di-
3,3'-(Iminodimethylene)dipyridine
Inchi: InChI=1S/C12H13N3/c1-3-11(7-13-5-1)9-15-10-12-4-2-6-14-8-12/h1-8,15H,9-10H2
InchiKey: FEBQXMFOLRVSGC-UHFFFAOYSA-N
Formula: C12H13N3
SMILES: c1cncc(CNCc2cccnc2)c1
Mol. weight [g/mol]: 199.26

Physical Properties

Property code	Value	Unit	Source
af	0.5191		Cheméo Relay (1.0)
gf	388.76	kJ/mol	Cheméo Relay (1.0, beta)
hf	277.50	kJ/mol	Cheméo Relay (1.0)
hvap	97.41	kJ/mol	Cheméo Relay (1.0)
ie	9.02	eV	Cheméo Relay (1.0)
log10ws	-0.48		Cheméo Relay (1.0)
logp	1.766		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
pc	3416.41	kPa	Cheméo Relay (1.0, beta)
tb	594.05	K	Cheméo Relay (1.0)
tc	864.83	K	Cheméo Relay (1.0)
tf	283.89	K	Cheméo Relay (1.0)
vc	0.595	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1656946&Units=SI
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):

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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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