1,8-NAPHTHYRIDINE

Other names: 1,8-Diazanaphthalene
1,8-Pyridopyridine
Inchi: InChI=1S/C8H6N2/c1-3-7-4-2-6-10-8(7)9-5-1/h1-6H
InchiKey: FLBAYUMRQUHISI-UHFFFAOYSA-N
Formula: C8H6N2
SMILES: c1cnc2ncccc2c1
Mol. weight [g/mol]: 130.15

Physical Properties

Property code	Value	Unit	Source
af	0.3758		Cheméo Relay (1.0)
gf	287.60	kJ/mol	Cheméo Relay (1.0, beta)
hf	248.44	kJ/mol	Cheméo Relay (1.0)
hvap	61.70	kJ/mol	Cheméo Relay (1.0)
ie	9.20	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-1.29		Cheméo Relay (1.0)
logp	1.630		Crippen Method
mcvol	100.320	ml/mol	McGowan Method
pc	5766.79	kPa	Cheméo Relay (1.0, beta)
tb	531.47	K	Cheméo Relay (1.0)
tc	790.22	K	Cheméo Relay (1.0)
tf	329.93	K	Cheméo Relay (1.0)
vc	0.372	m3/kmol	Cheméo Relay (1.0)

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=C254604&Units=SI

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