2-METHYLQUINOXILINE

Other names: 2-Methylquinoxaline
Inchi: InChI=1S/C9H8N2/c1-7-6-10-8-4-2-3-5-9(8)11-7/h2-6H,1H3
InchiKey: ALHUXMDEZNLFTA-UHFFFAOYSA-N
Formula: C9H8N2
SMILES: Cc1cnc2ccccc2n1
Mol. weight [g/mol]: 144.18

Physical Properties

Property code	Value	Unit	Source
af	0.4093		Cheméo Relay (1.0)
hf	205.27	kJ/mol	Cheméo Relay (1.0)
hvap	66.20	kJ/mol	Cheméo Relay (1.0)
ie	8.66	eV	Cheméo Relay (1.0)
log10ws	-1.27		Cheméo Relay (1.0)
logp	1.938		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
pc	4867.74	kPa	Cheméo Relay (1.0, beta)
rinpol	1272.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1272.00		NIST Webbook
ripol	1941.00		NIST Webbook
ripol	1936.00		NIST Webbook
ripol	1936.00		NIST Webbook
tb	519.20	K	NIST Webbook
tc	801.34	K	Cheméo Relay (1.0)
tf	317.92	K	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=C7251618&Units=SI

Legend

af:	Acentric Factor
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point