PYRIDINE, 4-METHYL-, 1-OXIDE

Other names:	4-Methylpyridine 1-oxide
	4-Methylpyridine N-oxide
	4-Picoline, 1-oxide
	4-methylpyridine-N-oxide
	4-picoline N-oxide
	«gamma»-Picoline 1-oxide
	«gamma»-Picoline N-oxide
Inchi:	InChI=1S/C6H7NO/c1-6-2-4-7(8)5-3-6/h2-5H,1H3
InchiKey:	IWYYIZOHWPCALJ-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cc1cc[n+]([O-])cc1
Mol. weight [g/mol]:	109.13

Physical Properties

Property code	Value	Unit	Source
af	0.3388		Cheméo Relay (1.0)
gf	207.56	kJ/mol	Cheméo Relay (1.0, beta)
hf	109.39	kJ/mol	Cheméo Relay (1.0)
hvap	62.29	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	0.06		Cheméo Relay (1.0)
logp	0.628		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
pc	4676.03	kPa	Cheméo Relay (1.0, beta)
tb	453.20	K	Cheméo Relay (1.0)
tc	658.94	K	Cheméo Relay (1.0)
tf	457.75	K	Thermal behaviour of nitrogen oxides relevant to oxidative denitrogenation
vc	0.283	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

Thermal behaviour of nitrogen oxides relevant to oxidative denitrogenation: https://www.doi.org/10.1016/j.jct.2019.04.014

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003674&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):	

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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