2,6-DIMETHOXYPYRIDINE

Inchi: InChI=1S/C7H9NO2/c1-9-6-4-3-5-7(8-6)10-2/h3-5H,1-2H3
InchiKey: IBTGEEMBZJBBSH-UHFFFAOYSA-N
Formula: C7H9NO2
SMILES: COc1cccc(OC)n1
Mol. weight [g/mol]: 139.15

Physical Properties

Property code	Value	Unit	Source
hf	-242.35	kJ/mol	Cheméo Relay (1.0)
hvap	55.35	kJ/mol	Cheméo Relay (1.0)
ie	8.66	eV	Cheméo Relay (1.0)
log10ws	-1.42		Cheméo Relay (1.0)
logp	1.099		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	3958.60	kPa	Cheméo Relay (1.0, beta)
rinpol	1028.10		NIST Webbook
tb	452.20	K	NIST Webbook
tf	289.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	53.90	kJ/mol	298.15	Thermochemistry of some methoxypyridines

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6231181&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):

Thermochemistry of some methoxypyridines: https://www.doi.org/10.1016/j.jct.2011.11.032

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point