Di(1-pyrazolyl)methane

Inchi: InChI=1S/C7H8N4/c1-3-8-10(5-1)7-11-6-2-4-9-11/h1-6H,7H2
InchiKey: WWNSYPVRCNOFJV-UHFFFAOYSA-N
Formula: C7H8N4
SMILES: c1cnn(Cn2cccn2)c1
Mol. weight [g/mol]: 148.17
CAS: 27258-04-4

Physical Properties

Property code	Value	Unit	Source
affp	924.70	kJ/mol	NIST Webbook
basg	893.90	kJ/mol	NIST Webbook
log10ws	-2.02		Crippen Method
logp	0.585		Crippen Method
mcvol	110.490	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27258044&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from: