1-methyl-3,5-diphenylpyrazole

Inchi: InChI=1S/C16H14N2/c1-18-16(14-10-6-3-7-11-14)12-15(17-18)13-8-4-2-5-9-13/h2-12H,1
InchiKey: SVDTUJAQNAQGGW-UHFFFAOYSA-N
Formula: C16H14N2
SMILES: Cn1nc(-c2ccccc2)cc1-c1ccccc1
Mol. weight [g/mol]: 234.30
CAS: 19311-79-6

Physical Properties

Property code	Value	Unit	Source
affp	958.90	kJ/mol	NIST Webbook
basg	927.00	kJ/mol	NIST Webbook
log10ws	-7.73		Crippen Method
logp	3.754		Crippen Method
mcvol	189.280	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	17.46	kJ/mol	220.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19311796&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume