3,3-Diphenyl-5-methyl-3h-pyrazole

Inchi: InChI=1S/C16H14N2/c1-13-12-16(18-17-13,14-8-4-2-5-9-14)15-10-6-3-7-11-15/h2-12H,1
InchiKey: RQPFXERQZHJWML-UHFFFAOYSA-N
Formula: C16H14N2
SMILES: CC1=CC(c2ccccc2)(c2ccccc2)N=N1
Mol. weight [g/mol]: 234.30

Physical Properties

Property code	Value	Unit	Source
hfus	25.25	kJ/mol	Joback Method
logp	4.300		Crippen Method
mcvol	189.280	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.66	J/mol×K	745.06	Joback Method
cpg	570.49	J/mol×K	793.80	Joback Method
cpg	588.89	J/mol×K	842.53	Joback Method
cpg	606.13	J/mol×K	891.27	Joback Method
cpg	622.53	J/mol×K	940.00	Joback Method
cpg	638.38	J/mol×K	988.74	Joback Method
cpg	653.98	J/mol×K	1037.47	Joback Method

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=C49716269&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume