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
CAS: 49716-26-9

Physical Properties

Property code	Value	Unit	Source
gf	623.57	kJ/mol	Joback Method
hf	421.24	kJ/mol	Joback Method
hfus	25.25	kJ/mol	Joback Method
hvap	68.53	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.300		Crippen Method
mcvol	189.280	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	745.06	K	Joback Method
tc	1037.47	K	Joback Method
tf	514.84	K	Joback Method
vc	0.725	m3/kmol	Joback 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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49716269&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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