2,5-Diphenyltetrazole

Other names: 2H-Tetrazole, 2,5-diphenyl-
2,5-Diphenyl-2H-tetrazole
2,5-Diphenyltetrazol
Inchi: InChI=1S/C13H10N4/c1-3-7-11(8-4-1)13-14-16-17(15-13)12-9-5-2-6-10-12/h1-10H
InchiKey: OJPYZWGULWNRSE-UHFFFAOYSA-N
Formula: C13H10N4
SMILES: c1ccc(-c2nnn(-c3ccccc3)n2)cc1
Mol. weight [g/mol]: 222.25
CAS: 18039-45-7

Physical Properties

Property code	Value	Unit	Source
chs	-6939.80 ± 2.10	kJ/mol	NIST Webbook
hf	515.10 ± 4.60	kJ/mol	NIST Webbook
hfs	395.00	kJ/mol	NIST Webbook
log10ws	-5.02		Crippen Method
logp	2.329		Crippen Method
mcvol	166.970	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	119.70	kJ/mol	333.00	NIST Webbook
hsubt	119.70 ± 4.20	kJ/mol	343.00	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=C18039457&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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