

p-Terphenyl, 4,4''-diamine

Other names:	4,4'-Diamino-p-terphenyl
Inchi:	InChI=1S/C18H16N2/c19-17-9-5-15(6-10-17)13-1-2-14(4-3-13)16-7-11-18(20)12-8-16/h1
InchiKey:	QBSMHWVGUPQNJJ-UHFFFAOYSA-N
Formula:	C18H16N2
SMILES:	<chem>Nc1ccc(-c2ccc(-c3ccc(N)cc3)cc2)cc1</chem>
Mol. weight [g/mol]:	260.33
CAS:	3365-85-3

Physical Properties

Property code	Value	Unit	Source
gf	541.92	kJ/mol	Joback Method
hf	327.91	kJ/mol	Joback Method
hfus	33.73	kJ/mol	Joback Method
hvap	85.76	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.185		Crippen Method
mcvol	213.160	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	851.28	K	Joback Method
tc	1128.34	K	Joback Method
tf	575.96	K	Joback Method
vc	0.777	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.12	J/molxK	851.28	Joback Method
cpg	628.35	J/molxK	897.46	Joback Method
cpg	641.20	J/molxK	943.63	Joback Method
cpg	652.80	J/molxK	989.81	Joback Method
cpg	663.29	J/molxK	1035.98	Joback Method
cpg	672.80	J/molxK	1082.16	Joback Method
cpg	681.46	J/molxK	1128.34	Joback Method

Sources

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=C3365853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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