4,4'-Diamino-p-terphenyl

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: Nc1ccc(-c2ccc(-c3ccc(N)cc3)cc2)cc1
Mol. weight [g/mol]: 260.34

Physical Properties

Property code	Value	Unit	Source
af	0.7337		Cheméo Relay (1.0)
gf	541.92	kJ/mol	Joback Method
hf	277.92	kJ/mol	Cheméo Relay (1.0)
hfus	33.73	kJ/mol	Joback Method
hvap	135.09	kJ/mol	Cheméo Relay (1.0)
ie	7.04	eV	Cheméo Relay (1.0)
log10ws	-4.96		Cheméo Relay (1.0)
logp	4.185		Crippen Method
mcvol	213.160	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	731.63	K	Cheméo Relay (1.0)
tc	1032.83	K	Cheméo Relay (1.0)
tf	459.03	K	Cheméo Relay (1.0)
vc	0.768	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3365853&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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