P,P'-(P-PHENYLENEDIOXY)DIANILINE

Other names: 1,4-Phenylene-di-4-aminophenyl ether
Benzenamine,4,4'-[1,4-phenylenebis(oxy)]bis-
Inchi: InChI=1S/C18H16N2O2/c19-13-1-5-15(6-2-13)21-17-9-11-18(12-10-17)22-16-7-3-14(20)
InchiKey: JCRRFJIVUPSNTA-UHFFFAOYSA-N
Formula: C18H16N2O2
SMILES: Nc1ccc(Oc2ccc(Oc3ccc(N)cc3)cc2)cc1
Mol. weight [g/mol]: 292.34

Physical Properties

Property code	Value	Unit	Source
af	0.8471		Cheméo Relay (1.0)
hf	22.47	kJ/mol	Cheméo Relay (1.0)
hfus	36.10	kJ/mol	Joback Method
hvap	128.64	kJ/mol	Cheméo Relay (1.0)
ie	6.60	eV	NIST Webbook
log10ws	-4.92		Cheméo Relay (1.0)
logp	4.436		Crippen Method
mcvol	224.900	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	721.33	K	Cheméo Relay (1.0)
tc	1036.17	K	Cheméo Relay (1.0)
tf	421.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.10	J/mol×K	896.12	Joback Method
cpg	677.74	J/mol×K	940.71	Joback Method
cpg	688.86	J/mol×K	985.29	Joback Method
cpg	698.53	J/mol×K	1029.88	Joback Method
cpg	706.80	J/mol×K	1074.46	Joback Method
cpg	713.75	J/mol×K	1119.05	Joback Method
cpg	719.42	J/mol×K	1163.63	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=C3491121&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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