4,4'-oxybis(benzene-1,2-diamine)

Other names: 3,3',4,4'-Tetraminodiphenyl ether
Inchi: InChI=1S/C12H14N4O/c13-9-3-1-7(5-11(9)15)17-8-2-4-10(14)12(16)6-8/h1-6H,13-16H2
InchiKey: RQBIGPMJQUKYAH-UHFFFAOYSA-N
Formula: C12H14N4O
SMILES: Nc1ccc(Oc2ccc(N)c(N)c2)cc1N
Mol. weight [g/mol]: 230.27
CAS: 2676-59-7

Physical Properties

Property code	Value	Unit	Source
chg	-6632.00 ± 2.00	kJ/mol	NIST Webbook
gf	397.26	kJ/mol	Joback Method
hf	139.11	kJ/mol	Joback Method
hfl	-91.00 ± 2.00	kJ/mol	NIST Webbook
hfus	35.34	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.808		Crippen Method
mcvol	178.210	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
ss	293.90	J/mol×K	NIST Webbook
ss	295.10	J/mol×K	NIST Webbook
tb	859.78	K	Joback Method
tc	1127.90	K	Joback Method
tf	683.19	K	Joback Method
tt	402.60 ± 0.10	K	NIST Webbook
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.49	J/mol×K	993.84	Joback Method
cpg	558.03	J/mol×K	1038.53	Joback Method
cpg	564.52	J/mol×K	1083.21	Joback Method

cpg	521.23	J/mol×K	859.78	Joback Method
cpg	532.13	J/mol×K	904.47	Joback Method
cpg	541.87	J/mol×K	949.15	Joback Method
cpg	570.02	J/mol×K	1127.90	Joback Method
cps	400.00	J/mol×K	300.00	NIST Webbook
cps	320.24	J/mol×K	300.00	NIST Webbook
hfust	25.30	kJ/mol	425.10	NIST Webbook
hfust	25.30	kJ/mol	402.60	NIST Webbook
sfust	62.80	J/mol×K	425.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2676597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

tt: Triple Point Temperature

vc: Critical Volume