4,4'-Oxydibenzonitrile

Other names:	Benzonitrile, 4,4'-oxybis-
	Benzonitrile, 4,4'-oxydi-
	4,4'-Dicyanodiphenyl ether
	Dibenzonitrile, 4,4'-oxy-
	cyclohex-4-ene-1,2-dicarboxylic anhydride
Inchi:	InChI=1S/C14H8N2O/c15-9-11-1-5-13(6-2-11)17-14-7-3-12(10-16)4-8-14/h1-8H
InchiKey:	RSAUOQFEFINEDM-UHFFFAOYSA-N
Formula:	C14H8N2O
SMILES:	N#Cc1ccc(Oc2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	220.23
CAS:	6508-04-9

Physical Properties

Property code	Value	Unit	Source
gf	433.92	kJ/mol	Joback Method
hf	315.37	kJ/mol	Joback Method
hfus	23.52	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.222		Crippen Method
mcvol	169.230	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
tb	809.62	K	Joback Method
tc	1068.92	K	Joback Method
tf	477.63	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.58	J/mol×K	809.62	Joback Method
cpg	443.46	J/mol×K	852.84	Joback Method
cpg	452.35	J/mol×K	896.05	Joback Method
cpg	460.29	J/mol×K	939.27	Joback Method

cpg	467.33	J/mol×K	982.49	Joback Method
cpg	473.50	J/mol×K	1025.71	Joback Method
cpg	478.87	J/mol×K	1068.92	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=C6508049&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