3,3'-Diamino-4,4'-dihydroxydiphenylmethane

Inchi: InChI=1S/C13H14N2O2/c14-10-6-8(1-3-12(10)16)5-9-2-4-13(17)11(15)7-9/h1-4,6-7,16-1
InchiKey: KCFVSHSJPIVGCG-UHFFFAOYSA-N
Formula: C13H14N2O2
SMILES: Nc1cc(Cc2ccc(O)c(N)c2)ccc1O
Mol. weight [g/mol]: 230.26
CAS: 6423-19-4

Physical Properties

Property code	Value	Unit	Source
gf	87.80	kJ/mol	Joback Method
hf	-148.57	kJ/mol	Joback Method
hfs	-335.00	kJ/mol	NIST Webbook
hfus	38.69	kJ/mol	Joback Method
hvap	97.72	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.853		Crippen Method
mcvol	178.210	ml/mol	McGowan Method
pc	4945.39	kPa	Joback Method
tb	866.46	K	Joback Method
tc	1135.62	K	Joback Method
tf	704.11	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.97	J/mol×K	866.46	Joback Method
cpg	540.00	J/mol×K	911.32	Joback Method
cpg	551.91	J/mol×K	956.18	Joback Method
cpg	563.94	J/mol×K	1001.04	Joback Method
cpg	576.34	J/mol×K	1045.90	Joback Method
cpg	589.32	J/mol×K	1090.76	Joback Method
cpg	603.13	J/mol×K	1135.62	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6423194&Units=SI&Mask=3FFF

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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