

Benzenamine, 3,3'-sulfonylbis-

Other names:

Aniline, 3,3'-sulfonyldi-
Bis(m-aminophenyl) sulfone
3,3'-Diaminodiphenyl sulfone
3,3'-Diaminophenyl sulfone
3,3'-Sulfonylbis(aniline)
3,3'-Sulfonyldianiline
Sulfone, bis(m-aminophenyl)
Sulfone, bis(3-aminophenyl)
3,3'-Diaminodifenylsulfon
3-Aminophenyl sulfone
3-Aminophenyl sulphone
NSC 20610
C 600
3,3'-sulphonyldianiline

Inchi:

InChI=1S/C12H12N2O2S/c13-9-3-1-5-11(7-9)17(15,16)12-6-2-4-10(14)8-12/h1-8H,13-14

InchiKey:

LJGHYPLBDBRCRZ-UHFFFAOYSA-N

Formula:

C12H12N2O2S

SMILES:

Nc1cccc(S(=O)(=O)c2cccc(N)c2)c1

Mol. weight [g/mol]:

248.30

CAS:

599-61-1

Physical Properties

Property code	Value	Unit	Source
gf	-79.92	kJ/mol	Joback Method
hf	-226.66	kJ/mol	Joback Method
hfus	35.91	kJ/mol	Joback Method
hvap	88.10	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.684		Crippen Method
mcvol	180.470	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
tb	730.12	K	Joback Method
tc	981.90	K	Joback Method
tf	507.96	K	Joback Method
vc	0.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.17	J/mol×K	730.12	Joback Method
cpg	487.20	J/mol×K	772.08	Joback Method
cpg	498.94	J/mol×K	814.05	Joback Method
cpg	509.42	J/mol×K	856.01	Joback Method
cpg	518.70	J/mol×K	897.97	Joback Method
cpg	526.81	J/mol×K	939.93	Joback Method
cpg	533.79	J/mol×K	981.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C599611&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

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

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