4-[(4-aminophenyl)sulfonylamino]benzenesulfona

Inchi: InChI=1S/C12H13N3O4S2/c13-9-1-5-12(6-2-9)21(18,19)15-10-3-7-11(8-4-10)20(14,16)1
InchiKey: GCQZFVAHUZIDRP-UHFFFAOYSA-N
Formula: C12H13N3O4S2
SMILES: Nc1ccc(S(=O)(=O)Nc2ccc(S(N)(=O)=O)cc2)cc1
Mol. weight [g/mol]: 327.39

Physical Properties

Property code	Value	Unit	Source
gf	-459.07	kJ/mol	Joback Method
hf	-626.54	kJ/mol	Joback Method
hfus	52.39	kJ/mol	Joback Method
hvap	113.17	kJ/mol	Joback Method
log10ws	-2.76		Aqueous Solubility Prediction Method
logp	0.717		Crippen Method
mcvol	218.540	ml/mol	McGowan Method
pc	5908.07	kPa	Joback Method
tb	828.07	K	Joback Method
tc	1066.32	K	Joback Method
tf	599.18	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.25	J/mol×K	828.07	Joback Method
cpg	617.81	J/mol×K	867.78	Joback Method
cpg	626.92	J/mol×K	907.49	Joback Method
cpg	634.58	J/mol×K	947.20	Joback Method
cpg	640.83	J/mol×K	986.91	Joback Method
cpg	645.67	J/mol×K	1026.61	Joback Method
cpg	649.11	J/mol×K	1066.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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