4-amino-N-(4-nitrophenyl)benzenesulfonamide

Inchi: InChI=1S/C12H11N3O4S/c13-9-1-7-12(8-2-9)20(18,19)14-10-3-5-11(6-4-10)15(16)17/h1
InchiKey: ACJNABKXDUDYAM-UHFFFAOYSA-N
Formula: C12H11N3O4S
SMILES: Nc1ccc(S(=O)(=O)Nc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 293.30

Physical Properties

Property code	Value	Unit	Source
gf	-21.43	kJ/mol	Joback Method
hf	-217.74	kJ/mol	Joback Method
hfus	27.90	kJ/mol	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
hfus	27.90 ± 0.50	kJ/mol	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
hvap	100.48	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	1.978		Crippen Method
mcvol	197.890	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
tb	859.60	K	Joback Method
tc	1119.77	K	Joback Method
tf	438.90	K	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
tf	439.00 ± 0.20	K	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.24	J/mol×K	859.60	Joback Method
cpg	566.19	J/mol×K	902.96	Joback Method
cpg	574.78	J/mol×K	946.32	Joback Method
cpg	582.06	J/mol×K	989.69	Joback Method
cpg	588.10	J/mol×K	1033.05	Joback Method
cpg	592.93	J/mol×K	1076.41	Joback Method
cpg	596.62	J/mol×K	1119.77	Joback Method
psub	4.01e-06	kPa	417.25	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.18e-06	kPa	409.45	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.30e-06	kPa	412.85	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	3.41e-06	kPa	415.15	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.50e-06	kPa	405.55	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	4.34e-06	kPa	418.75	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides

psub	5.46e-06	kPa	420.05	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	5.63e-06	kPa	421.55	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	6.16e-06	kPa	423.25	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	7.30e-06	kPa	424.65	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	8.92e-06	kPa	426.25	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.05e-05	kPa	428.75	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.28e-05	kPa	431.35	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides

psub	1.41e-05	kPa	432.05	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.81e-05	kPa	435.15	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.28e-05	kPa	438.25	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides:	https://www.doi.org/10.1016/j.jct.2010.12.007
Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents:	https://www.doi.org/10.1021/je500918t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
psub:	Sublimation pressure

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume