4-amino-N-(4-cyanophenyl)benzenesulfonamide

Inchi: InChI=1S/C13H11N3O2S/c14-9-10-1-5-12(6-2-10)16-19(17,18)13-7-3-11(15)4-8-13/h1-8
InchiKey: PLPNDNWDSGFETI-UHFFFAOYSA-N
Formula: C13H11N3O2S
SMILES: N#Cc1ccc(NS(=O)(=O)c2ccc(N)cc2)cc1
Mol. weight [g/mol]: 273.32

Physical Properties

Property code	Value	Unit	Source
gf	84.62	kJ/mol	Joback Method
hf	-62.74	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
hfus	30.90 ± 0.50	kJ/mol	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
hvap	96.60	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	1.941		Crippen Method
mcvol	195.940	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	832.72	K	Joback Method
tc	1081.12	K	Joback Method
tf	451.50	K	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
tf	451.60 ± 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	531.98	J/mol×K	832.72	Joback Method
cpg	542.06	J/mol×K	874.12	Joback Method
cpg	550.93	J/mol×K	915.52	Joback Method
cpg	558.64	J/mol×K	956.92	Joback Method
cpg	565.21	J/mol×K	998.32	Joback Method
cpg	570.69	J/mol×K	1039.72	Joback Method
cpg	575.13	J/mol×K	1081.12	Joback Method
psub	1.36e-05	kPa	426.55	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	7.23e-06	kPa	420.95	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	7.91e-06	kPa	421.35	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.13e-05	kPa	424.75	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	6.74e-06	kPa	420.15	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.66e-05	kPa	428.35	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides

psub	1.94e-05	kPa	429.65	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.11e-05	kPa	431.35	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.28e-05	kPa	431.75	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.33e-05	kPa	432.35	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.63e-05	kPa	433.05	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	3.17e-05	kPa	434.75	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	3.58e-05	kPa	435.75	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides

psub	4.24e-05	kPa	437.15	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	4.37e-05	kPa	437.55	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

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