4-amino-N-(4-chlorophenyl)benzenesulfonamide

Inchi: InChI=1S/C12H11ClN2O2S/c13-9-1-5-11(6-2-9)15-18(16,17)12-7-3-10(14)4-8-12/h1-8,15
InchiKey: RBJGYDGKXTYSSL-UHFFFAOYSA-N
Formula: C12H11ClN2O2S
SMILES: Nc1ccc(S(=O)(=O)Nc2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 282.75

Physical Properties

Property code	Value	Unit	Source
gf	-68.91	kJ/mol	Joback Method
hf	-222.72	kJ/mol	Joback Method
hfus	23.80 ± 0.50	kJ/mol	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
hvap	88.28	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.723		Crippen Method
mcvol	192.710	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	745.19	K	Joback Method
tc	991.17	K	Joback Method
tf	467.90 ± 0.20	K	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.22	J/mol×K	745.19	Joback Method
cpg	501.37	J/mol×K	786.19	Joback Method
cpg	512.29	J/mol×K	827.18	Joback Method
cpg	522.01	J/mol×K	868.18	Joback Method
cpg	530.58	J/mol×K	909.17	Joback Method

cpg	538.03	J/mol×K	950.17	Joback Method
cpg	544.41	J/mol×K	991.17	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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