4-amino-N,N-dimethylbenzenesulfonamide

Inchi: InChI=1S/C8H12N2O2S/c1-10(2)13(11,12)8-5-3-7(9)4-6-8/h3-6H,9H2,1-2H3
InchiKey: BABGMPQXLCJMSK-UHFFFAOYSA-N
Formula: C8H12N2O2S
SMILES: CN(C)S(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 200.26

Physical Properties

Property code	Value	Unit	Source
gf	-172.05	kJ/mol	Joback Method
hf	-335.42	kJ/mol	Joback Method
hfus	29.70 ± 0.50	kJ/mol	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
hvap	67.66	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.519		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
tb	546.85	K	Joback Method
tc	759.56	K	Joback Method
tf	444.60 ± 0.20	K	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.12	J/mol×K	546.85	Joback Method
cpg	352.78	J/mol×K	582.30	Joback Method
cpg	365.58	J/mol×K	617.75	Joback Method
cpg	377.54	J/mol×K	653.20	Joback Method
cpg	388.66	J/mol×K	688.65	Joback Method

cpg	398.98	J/mol×K	724.10	Joback Method
cpg	408.51	J/mol×K	759.56	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

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