4-amino-N-methylbenzenesulfonamide

Inchi: InChI=1S/C7H10N2O2S/c1-9-12(10,11)7-4-2-6(8)3-5-7/h2-5,9H,8H2,1H3
InchiKey: OISQSDKFWKJEBA-UHFFFAOYSA-N
Formula: C7H10N2O2S
SMILES: CNS(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 186.24

Physical Properties

Property code	Value	Unit	Source
gf	-201.86	kJ/mol	Joback Method
hf	-328.84	kJ/mol	Joback Method
hfus	17.10 ± 0.50	kJ/mol	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
hvap	69.83	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.177		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
pc	5495.11	kPa	Joback Method
tb	561.70	K	Joback Method
tc	781.20	K	Joback Method
tf	382.20 ± 0.20	K	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.65	J/mol×K	561.70	Joback Method
cpg	317.73	J/mol×K	598.28	Joback Method
cpg	329.03	J/mol×K	634.87	Joback Method
cpg	339.56	J/mol×K	671.45	Joback Method
cpg	349.32	J/mol×K	708.03	Joback Method

cpg	358.33	J/mol×K	744.61	Joback Method
cpg	366.60	J/mol×K	781.20	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