

4-amino-N-(4-methoxyphenyl)benzenesulfonamid

Inchi:	InChI=1S/C13H14N2O3S/c1-18-12-6-4-11(5-7-12)15-19(16,17)13-8-2-10(14)3-9-13/h2-9
InchiKey:	PKCILPHWDZXVQT-UHFFFAOYSA-N
Formula:	C13H14N2O3S
SMILES:	COc1ccc(NS(=O)(=O)c2ccc(N)cc2)cc1
Mol. weight [g/mol]:	278.33

Physical Properties

Property code	Value	Unit	Source
gf	-153.56	kJ/mol	Joback Method
hf	-359.84	kJ/mol	Joback Method
hfus	38.60 ± 0.50	kJ/mol	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
hvap	88.53	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.078		Crippen Method
mcvol	200.430	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	753.06	K	Joback Method
tc	988.51	K	Joback Method
tf	467.40 ± 0.20	K	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.69	J/molxK	753.06	Joback Method
cpg	557.12	J/molxK	792.30	Joback Method
cpg	569.28	J/molxK	831.54	Joback Method
cpg	580.19	J/molxK	870.78	Joback Method
cpg	589.86	J/molxK	910.02	Joback Method

cpg	598.32	J/mol×K	949.27	Joback Method
cpg	605.57	J/mol×K	988.51	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/ci990307i>

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

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