Benzenesulfonamide, 4-amino-N-(4-methoxyphenyl)-

Other names: N1-(4-Methoxyphenyl)sulfanilamide
p-Sulphanilanisidide
4-Amino-N-(4-methoxyphenyl)benzenesulfonamide

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

CAS: 19837-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-153.56	kJ/mol	Joback Method
hf	-359.84	kJ/mol	Joback Method
hfus	39.59	kJ/mol	Joback Method
hsub	124.00 ± 1.00	kJ/mol	NIST Webbook
hvap	99.40	kJ/mol	NIST Webbook
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	510.86	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	598.32	J/mol×K	949.27	Joback Method
cpg	605.57	J/mol×K	988.51	Joback Method
hfust	38.60	kJ/mol	467.40	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19837742&Units=SI
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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