Benzenesulfonamide, 5-amino-2-methyl-N-phenyl-

Other names: o-Toluenesulfonanilide, 5-amino-
5-Amino-o-toluenesulfonanilide
5-Amino-2-toluenesulfonanilide
5-Amino-ortho-toluenesulfonanilide
4-aminotoluene-2-sulphonanilide

Inchi: InChI=1S/C13H14N2O2S/c1-10-7-8-11(14)9-13(10)18(16,17)15-12-5-3-2-4-6-12/h2-9,15

InchiKey: HCAKHJQTCPZXPR-UHFFFAOYSA-N

Formula: C13H14N2O2S

SMILES: Cc1ccc(N)cc1S(=O)(=O)Nc1ccccc1

Mol. weight [g/mol]: 262.33

CAS: 79-72-1

Physical Properties

Property code	Value	Unit	Source
gf	-48.56	kJ/mol	Joback Method
hf	-227.62	kJ/mol	Joback Method
hfus	38.40	kJ/mol	Joback Method
hvap	86.12	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.378		Crippen Method
mcvol	194.560	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
tb	730.64	K	Joback Method
tc	969.46	K	Joback Method
tf	488.63	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.24	J/mol×K	730.64	Joback Method
cpg	532.17	J/mol×K	770.44	Joback Method
cpg	544.83	J/mol×K	810.25	Joback Method
cpg	556.26	J/mol×K	850.05	Joback Method

cpg	566.50	J/mol×K	889.86	Joback Method
cpg	575.60	J/mol×K	929.66	Joback Method
cpg	583.58	J/mol×K	969.46	Joback Method

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=C79721&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
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