4-Amino-n, n-dimethyl-2-phenylsulfonylaniline

Inchi: InChI=1S/C14H16N2O2S/c1-16(2)13-9-8-11(15)10-14(13)19(17,18)12-6-4-3-5-7-12/h3-1
InchiKey: SXSWLMBQTSJDAX-UHFFFAOYSA-N
Formula: C14H16N2O2S
SMILES: CN(C)c1ccc(N)cc1S(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 276.35
CAS: 19770-99-1

Physical Properties

Property code	Value	Unit	Source
gf	-18.75	kJ/mol	Joback Method
hf	-234.20	kJ/mol	Joback Method
hfus	38.92	kJ/mol	Joback Method
hvap	83.95	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.168		Crippen Method
mcvol	208.650	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	715.79	K	Joback Method
tc	948.81	K	Joback Method
tf	479.71	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.04	J/mol×K	715.79	Joback Method
cpg	573.35	J/mol×K	754.63	Joback Method
cpg	587.33	J/mol×K	793.46	Joback Method
cpg	600.06	J/mol×K	832.30	Joback Method
cpg	611.57	J/mol×K	871.14	Joback Method
cpg	621.92	J/mol×K	909.98	Joback Method
cpg	631.15	J/mol×K	948.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C19770991&Units=SI

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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