P-(p-tolylsulfonylamido-)diphenylamine

Other names: 4'-anilinotoluene-4-sulphonanilide
Inchi: InChI=1S/C19H18N2O2S/c1-15-7-13-19(14-8-15)24(22,23)21-18-11-9-17(10-12-18)20-1
InchiKey: KEZPMZSDLBJCHH-UHFFFAOYSA-N
Formula: C19H18N2O2S
SMILES: Cc1ccc(S(=O)(=O)Nc2ccc(Nc3ccccc3)cc2)cc1
Mol. weight [g/mol]: 338.42
CAS: 100-93-6

Physical Properties

Property code	Value	Unit	Source
gf	137.31	kJ/mol	Joback Method
hf	-95.25	kJ/mol	Joback Method
hfus	47.89	kJ/mol	Joback Method
hvap	97.55	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.539		Crippen Method
mcvol	255.340	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	872.24	K	Joback Method
tc	1117.68	K	Joback Method
tf	552.07	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.84	J/mol×K	872.24	Joback Method
cpg	757.29	J/mol×K	913.15	Joback Method
cpg	769.22	J/mol×K	954.05	Joback Method
cpg	779.71	J/mol×K	994.96	Joback Method
cpg	788.85	J/mol×K	1035.87	Joback Method
cpg	796.70	J/mol×K	1076.77	Joback Method
cpg	803.37	J/mol×K	1117.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100936&Units=SI
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

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