Aniline, 4-(n,n-diethylamino)-2-(p-tolylsulfonyl)-

Inchi: InChI=1S/C17H22N2O2S/c1-4-19(5-2)14-8-11-16(18)17(12-14)22(20,21)15-9-6-13(3)7-1

InchiKey: ZHQDEKYRCTUNAM-UHFFFAOYSA-N

Formula: C17H22N2O2S

SMILES: CCN(CC)c1ccc(N)c(S(=O)(=O)c2ccc(C)cc2)c1

Mol. weight [g/mol]: 318.43

CAS: 19770-83-3

Physical Properties

Property code	Value	Unit	Source
gf	-3.12	kJ/mol	Joback Method
hf	-307.59	kJ/mol	Joback Method
hfus	46.30	kJ/mol	Joback Method
hvap	91.29	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.256		Crippen Method
mcvol	250.920	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
tb	789.41	K	Joback Method
tc	1012.04	K	Joback Method
tf	526.04	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.92	J/mol×K	789.41	Joback Method
cpg	736.62	J/mol×K	826.51	Joback Method
cpg	751.01	J/mol×K	863.62	Joback Method
cpg	764.14	J/mol×K	900.72	Joback Method
cpg	776.05	J/mol×K	937.83	Joback Method
cpg	786.81	J/mol×K	974.93	Joback Method
cpg	796.44	J/mol×K	1012.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19770833&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

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