Aniline, 4-(n,n-diethylamino)-2-(3,4-dimethylphenylsulfony

Inchi: InChI=1S/C18H24N2O2S/c1-5-20(6-2)15-8-10-17(19)18(12-15)23(21,22)16-9-7-13(3)14(

InchiKey: PDEAWBLBKIJMCJ-UHFFFAOYSA-N

Formula: C18H24N2O2S

SMILES: CCN(CC)c1ccc(N)c(S(=O)(=O)c2ccc(C)c(C)c2)c1

Mol. weight [g/mol]: 332.46

CAS: 19789-55-0

Physical Properties

Property code	Value	Unit	Source
gf	-4.33	kJ/mol	Joback Method
hf	-339.70	kJ/mol	Joback Method
hfus	48.50	kJ/mol	Joback Method
hvap	94.18	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.565		Crippen Method
mcvol	265.010	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
tb	817.27	K	Joback Method
tc	1037.99	K	Joback Method
tf	549.83	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.60	J/mol×K	817.27	Joback Method
cpg	792.27	J/mol×K	854.06	Joback Method
cpg	806.63	J/mol×K	890.84	Joback Method
cpg	819.73	J/mol×K	927.63	Joback Method
cpg	831.61	J/mol×K	964.42	Joback Method
cpg	842.31	J/mol×K	1001.20	Joback Method
cpg	851.87	J/mol×K	1037.99	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=C19789550&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