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

Inchi: InChI=1S/C17H19N3O2S/c1-3-20(4-2)14-7-10-16(19)17(11-14)23(21,22)15-8-5-13(12-18

InchiKey: REEQRZIJIABFCS-UHFFFAOYSA-N

Formula: C17H19N3O2S

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

Mol. weight [g/mol]: 329.42

CAS: 19789-56-1

Physical Properties

Property code	Value	Unit	Source
gf	130.06	kJ/mol	Joback Method
hf	-142.71	kJ/mol	Joback Method
hfus	47.80	kJ/mol	Joback Method
hvap	101.77	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.819		Crippen Method
mcvol	252.300	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
tb	891.49	K	Joback Method
tc	1125.08	K	Joback Method
tf	591.03	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.01	J/mol×K	891.49	Joback Method
cpg	751.85	J/mol×K	930.42	Joback Method
cpg	762.43	J/mol×K	969.35	Joback Method
cpg	771.81	J/mol×K	1008.29	Joback Method
cpg	780.04	J/mol×K	1047.22	Joback Method
cpg	787.17	J/mol×K	1086.15	Joback Method
cpg	793.26	J/mol×K	1125.08	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=C19789561&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