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

Inchi: InChI=1S/C16H19ClN2O2S/c1-3-19(4-2)13-7-10-15(18)16(11-13)22(20,21)14-8-5-12(17)

InchiKey: TYVKQKGYFZFZSL-UHFFFAOYSA-N

Formula: C16H19ClN2O2S

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

Mol. weight [g/mol]: 338.85

CAS: 19789-54-9

Physical Properties

Property code	Value	Unit	Source
gf	-23.47	kJ/mol	Joback Method
hf	-302.69	kJ/mol	Joback Method
hfus	47.90	kJ/mol	Joback Method
hvap	93.45	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.601		Crippen Method
mcvol	249.070	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	803.96	K	Joback Method
tc	1032.54	K	Joback Method
tf	544.69	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.58	J/mol×K	803.96	Joback Method
cpg	704.69	J/mol×K	842.06	Joback Method
cpg	717.52	J/mol×K	880.15	Joback Method
cpg	729.13	J/mol×K	918.25	Joback Method
cpg	739.55	J/mol×K	956.35	Joback Method
cpg	748.85	J/mol×K	994.44	Joback Method
cpg	757.06	J/mol×K	1032.54	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=C19789549&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