

Aniline, n,n-diethyl-p-(p-tolylsulfonamido)-

Inchi:	InChI=1S/C17H22N2O2S/c1-4-19(5-2)16-10-8-15(9-11-16)18-22(20,21)17-12-6-14(3)7-1
InchiKey:	ONDXXZIDUKAMOL-UHFFFAOYSA-N
Formula:	C17H22N2O2S
SMILES:	CCN(CC)c1ccc(NS(=O)(=O)c2ccc(C)cc2)cc1
Mol. weight [g/mol]:	318.43
CAS:	19770-76-4

Physical Properties

Property code	Value	Unit	Source
gf	29.45	kJ/mol	Joback Method
hf	-276.44	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	86.43	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.642		Crippen Method
mcvol	250.920	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
tb	762.07	K	Joback Method
tc	977.42	K	Joback Method
tf	482.92	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.58	J/molxK	762.07	Joback Method
cpg	727.95	J/molxK	797.96	Joback Method
cpg	743.02	J/molxK	833.85	Joback Method
cpg	756.85	J/molxK	869.75	Joback Method
cpg	769.49	J/molxK	905.64	Joback Method
cpg	780.99	J/molxK	941.53	Joback Method
cpg	791.39	J/molxK	977.42	Joback Method

Sources

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=C19770764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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