

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

Inchi:	InChI=1S/C15H18N2O2S/c1-11-4-7-13(8-5-11)20(18,19)15-10-12(17(2)3)6-9-14(15)16/h
InchiKey:	GWHVLJHWAVVOJZ-UHFFFAOYSA-N
Formula:	C15H18N2O2S
SMILES:	Cc1ccc(S(=O)(=O)c2cc(N(C)C)ccc2N)cc1
Mol. weight [g/mol]:	290.38
CAS:	19789-51-6

Physical Properties

Property code	Value	Unit	Source
gf	-19.96	kJ/mol	Joback Method
hf	-266.31	kJ/mol	Joback Method
hfus	41.12	kJ/mol	Joback Method
hvap	86.84	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.476		Crippen Method
mcvol	222.740	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	743.65	K	Joback Method
tc	973.25	K	Joback Method
tf	503.50	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.60	J/molxK	743.65	Joback Method
cpg	625.99	J/molxK	781.92	Joback Method
cpg	640.07	J/molxK	820.18	Joback Method
cpg	652.91	J/molxK	858.45	Joback Method
cpg	664.54	J/molxK	896.72	Joback Method
cpg	675.01	J/molxK	934.98	Joback Method
cpg	684.36	J/molxK	973.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C19789516&Units=SI

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
mccvol:	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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