

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

Inchi:	InChI=1S/C14H15ClN2O2S/c1-17(2)11-5-8-13(16)14(9-11)20(18,19)12-6-3-10(15)4-7-12
InchiKey:	XKUYLCRQBNOEME-UHFFFAOYSA-N
Formula:	C14H15ClN2O2S
SMILES:	CN(C)c1ccc(N)c(S(=O)(=O)c2ccc(Cl)cc2)c1
Mol. weight [g/mol]:	310.80
CAS:	19770-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-40.31	kJ/mol	Joback Method
hf	-261.41	kJ/mol	Joback Method
hfus	42.72	kJ/mol	Joback Method
hvap	89.00	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.821		Crippen Method
mcvol	220.890	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	758.20	K	Joback Method
tc	994.46	K	Joback Method
tf	522.15	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.80	J/molxK	758.20	Joback Method
cpg	595.50	J/molxK	797.58	Joback Method
cpg	607.93	J/molxK	836.95	Joback Method
cpg	619.14	J/molxK	876.33	Joback Method
cpg	629.18	J/molxK	915.71	Joback Method
cpg	638.09	J/molxK	955.08	Joback Method
cpg	645.91	J/molxK	994.46	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=C19770811&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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