2-Methoxyaniline-5-sulfonic acid diethylamide

Other names:	N',N'-Diethyl-3-amino-4-methoxybenzenesulfonamide
	Fast Red ITR Base
	Benzenesulfonamide, 3-amino-N,N-diethyl-4-methoxy-
	Azoic diazo component 42, base
	Brentamine Fast Red ITR Base
	C.I. 37150
	Metanilamide, N1,N1-diethyl-4-methoxy-
	N1,N1-Diethyl-4-methoxymetanilamide
	Orle Base Fast Red ITR
	Red ITR base
	2-Methoxy-5-(diethylaminosulfonyl)aniline
	2-Methoxy-5-(diethylsulfamoyl)aniline
	2-Methoxy-5-(N,N-diethylsulfamoyl)aniline
	NSC 50670
	3-amino-N,N-diethyl-4-methoxybenzenesulphonamide
Inchi:	InChI=1S/C11H18N2O3S/c1-4-13(5-2)17(14,15)9-6-7-11(16-3)10(12)8-9/h6-8H,4-5,12H2
InchiKey:	WBGVVXSCGNGJFL-UHFFFAOYSA-N
Formula:	C11H18N2O3S
SMILES:	CCN(CC)S(=O)(=O)c1ccc(OC)c(N)c1
Mol. weight [g/mol]:	258.34
CAS:	97-35-8

Physical Properties

Property code	Value	Unit	Source
gf	-261.42	kJ/mol	Joback Method
hf	-541.03	kJ/mol	Joback Method
hfus	38.29	kJ/mol	Joback Method
hvap	77.41	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.308		Crippen Method
mcvol	196.010	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	642.89	K	Joback Method
tc	844.88	K	Joback Method
tf	441.71	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.01	J/mol×K	642.89	Joback Method
cpg	525.01	J/mol×K	676.56	Joback Method
cpg	539.11	J/mol×K	710.22	Joback Method
cpg	552.31	J/mol×K	743.89	Joback Method
cpg	564.62	J/mol×K	777.55	Joback Method
cpg	576.04	J/mol×K	811.22	Joback Method
cpg	586.58	J/mol×K	844.88	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=C97358&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