N'-ethyl-4-phenoxymetanilanilide

Other names: 3-amino-N-ethyl-4-phenoxy-N-phenylbenzenesulphonamide
Inchi: InChI=1S/C20H20N2O3S/c1-2-22(16-9-5-3-6-10-16)26(23,24)18-13-14-20(19(21)15-18)
InchiKey: GHUSPTPILIZGPQ-UHFFFAOYSA-N
Formula: C20H20N2O3S
SMILES: CCN(c1ccccc1)S(=O)(=O)c1ccc(Oc2ccccc2)c(N)c1
Mol. weight [g/mol]: 368.45
CAS: 51929-55-6

Physical Properties

Property code	Value	Unit	Source
gf	39.18	kJ/mol	Joback Method
hf	-253.73	kJ/mol	Joback Method
hfus	49.68	kJ/mol	Joback Method
hvap	102.00	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.276		Crippen Method
mcvol	275.300	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
tb	902.17	K	Joback Method
tc	1146.47	K	Joback Method
tf	595.98	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.29	J/mol×K	902.17	Joback Method
cpg	835.45	J/mol×K	942.89	Joback Method
cpg	847.00	J/mol×K	983.60	Joback Method
cpg	857.03	J/mol×K	1024.32	Joback Method
cpg	865.61	J/mol×K	1065.04	Joback Method
cpg	872.80	J/mol×K	1105.75	Joback Method
cpg	878.70	J/mol×K	1146.47	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=C51929556&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