2-Ethoxy-5-nitroaniline

Inchi: InChI=1S/C8H10N2O3/c1-2-13-8-4-3-6(10(11)12)5-7(8)9/h3-5H,2,9H2,1H3
InchiKey: AMMPGYPPRLWMLW-UHFFFAOYSA-N
Formula: C8H10N2O3
SMILES: CCOc1ccc([N+](=O)[O-])cc1N
Mol. weight [g/mol]: 182.18

Physical Properties

Property code	Value	Unit	Source
gf	106.63	kJ/mol	Joback Method
hf	-104.05	kJ/mol	Joback Method
hfus	27.49	kJ/mol	Joback Method
hvap	66.64	kJ/mol	Joback Method
log10ws	-3.21		Aqueous Solubility Prediction Method
logp	1.576		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	665.87	K	Joback Method
tc	914.06	K	Joback Method
tf	369.65	K	Aqueous Solubility Prediction Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.87	J/mol×K	665.87	Joback Method
cpg	350.29	J/mol×K	707.23	Joback Method
cpg	360.88	J/mol×K	748.60	Joback Method
cpg	370.64	J/mol×K	789.96	Joback Method
cpg	379.60	J/mol×K	831.33	Joback Method
cpg	387.78	J/mol×K	872.69	Joback Method
cpg	395.18	J/mol×K	914.06	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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