5-Nitro-2-propoxyaniline

Inchi: InChI=1S/C9H12N2O3/c1-2-5-14-9-4-3-7(11(12)13)6-8(9)10/h3-4,6H,2,5,10H2,1H3
InchiKey: RXQCEGOUSFBKPI-UHFFFAOYSA-N
Formula: C9H12N2O3
SMILES: CCCOc1ccc([N+](=O)[O-])cc1N
Mol. weight [g/mol]: 196.21

Physical Properties

Property code	Value	Unit	Source
gf	115.05	kJ/mol	Joback Method
hf	-124.69	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	68.87	kJ/mol	Joback Method
log10ws	-3.16		Aqueous Solubility Prediction Method
logp	1.966		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	688.75	K	Joback Method
tc	931.55	K	Joback Method
tf	491.75	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.90	J/mol×K	688.75	Joback Method
cpg	400.07	J/mol×K	729.22	Joback Method
cpg	411.36	J/mol×K	769.68	Joback Method
cpg	421.79	J/mol×K	810.15	Joback Method
cpg	431.38	J/mol×K	850.62	Joback Method
cpg	440.13	J/mol×K	891.09	Joback Method
cpg	448.08	J/mol×K	931.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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