2-(2-Nitrophenoxy)acetic acid

Inchi: InChI=1S/C8H7NO5/c10-8(11)5-14-7-4-2-1-3-6(7)9(12)13/h1-4H,5H2,(H,10,11)
InchiKey: TYHHDWAHJRRYCU-UHFFFAOYSA-N
Formula: C8H7NO5
SMILES: O=C(O)COc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 197.15

Physical Properties

Property code	Value	Unit	Source
gf	-215.93	kJ/mol	Joback Method
hf	-391.18	kJ/mol	Joback Method
hfus	28.36	kJ/mol	Joback Method
hvap	78.77	kJ/mol	Joback Method
log10ws	-2.01		Aqueous Solubility Prediction Method
logp	1.058		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
tb	734.41	K	Joback Method
tc	961.16	K	Joback Method
tf	495.45	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.57	J/mol×K	734.41	Joback Method
cpg	346.85	J/mol×K	772.20	Joback Method
cpg	354.44	J/mol×K	809.99	Joback Method
cpg	361.38	J/mol×K	847.78	Joback Method
cpg	367.66	J/mol×K	885.57	Joback Method
cpg	373.32	J/mol×K	923.37	Joback Method
cpg	378.35	J/mol×K	961.16	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