2-Nitrophenol, isoBOC

Inchi: InChI=1S/C11H13NO5/c1-8(2)7-16-11(13)17-10-6-4-3-5-9(10)12(14)15/h3-6,8H,7H2,1-2
InchiKey: BGWYBIDQVQFSLX-UHFFFAOYSA-N
Formula: C11H13NO5
SMILES: CC(C)COC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 239.22

Physical Properties

Property code	Value	Unit	Source
gf	-161.29	kJ/mol	Joback Method
hf	-438.37	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.766		Crippen Method
mcvol	172.820	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1726.00		NIST Webbook
tb	732.85	K	Joback Method
tc	966.70	K	Joback Method
tf	475.67	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.00	J/mol×K	732.85	Joback Method
cpg	483.69	J/mol×K	771.82	Joback Method
cpg	495.38	J/mol×K	810.80	Joback Method
cpg	506.06	J/mol×K	849.77	Joback Method
cpg	515.76	J/mol×K	888.75	Joback Method
cpg	524.47	J/mol×K	927.72	Joback Method
cpg	532.21	J/mol×K	966.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume