4-Nitrophenol, isoBOC

Other names: 4-Nitrophenol, isoBOC
Inchi: InChI=1S/C11H13NO5/c1-8(2)7-16-11(13)17-10-5-3-9(4-6-10)12(14)15/h3-6,8H,7H2,1-2
InchiKey: WLRSOECSWRWZTI-UHFFFAOYSA-N
Formula: C11H13NO5
SMILES: CC(C)COC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 239.23

Physical Properties

Property code	Value	Unit	Source
hf	-513.32	kJ/mol	Cheméo Relay (1.0)
hfus	29.71	kJ/mol	Joback Method
hvap	88.42	kJ/mol	Cheméo Relay (1.0)
ie	9.47	eV	Cheméo Relay (1.0)
log10ws	-3.88		Cheméo Relay (1.0)
logp	2.766		Crippen Method
mcvol	172.820	ml/mol	McGowan Method
rinpol	1820.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	578.99	K	Cheméo Relay (1.0)
tf	331.76	K	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357838&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point