2-Amino-4-nitrophenol, N-acetyl-

Inchi: InChI=1S/C8H8N2O4/c1-5(11)9-7-4-6(10(13)14)2-3-8(7)12/h2-4,12H,1H3,(H,9,11)
InchiKey: GFHYFPARONGSCD-UHFFFAOYSA-N
Formula: C8H8N2O4
SMILES: CC(=O)Nc1cc([N+](=O)[O-])ccc1O
Mol. weight [g/mol]: 196.16

Physical Properties

Property code	Value	Unit	Source
gf	-39.34	kJ/mol	Joback Method
hf	-230.57	kJ/mol	Joback Method
hfus	33.97	kJ/mol	Joback Method
hvap	79.13	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.259		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	4869.76	kPa	Joback Method
rinpol	2111.00		NIST Webbook
rinpol	2111.00		NIST Webbook
tb	750.60	K	Joback Method
tc	1005.88	K	Joback Method
tf	576.78	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.98	J/mol×K	750.60	Joback Method
cpg	368.01	J/mol×K	793.15	Joback Method
cpg	376.41	J/mol×K	835.69	Joback Method
cpg	384.30	J/mol×K	878.24	Joback Method
cpg	391.79	J/mol×K	920.79	Joback Method
cpg	398.99	J/mol×K	963.34	Joback Method
cpg	406.01	J/mol×K	1005.88	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374267&Units=SI

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

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