

4-amino-2-nitrophenol

Inchi:	InChI=1S/C6H6N2O3/c7-4-1-2-6(9)5(3-4)8(10)11/h1-3,9H,7H2
InchiKey:	WHODQVWERNSQEO-UHFFFAOYSA-N
Formula:	C6H6N2O3
SMILES:	Nc1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	154.13
CAS:	119-34-6

Physical Properties

Property code	Value	Unit	Source
hf	-99.65	kJ/mol	Cheméo Relay (1.0)
hfus	27.29	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Cheméo Relay (1.0)
ie	7.95	eV	Cheméo Relay (1.0)
log10ws	-1.92		Cheméo Relay (1.0)
logp	0.883		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
tb	571.23	K	Cheméo Relay (1.0)
tf	400.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.91100e+01
Coeff. B	7.51260e-01
Coeff. C	-6.44920e-04
Coeff. D	2.24700e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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