

2-Amino-4-nitrophenol, N,O-bis(methyl)-

Inchi:	InChI=1S/C8H10N2O3/c1-9-7-5-6(10(11)12)3-4-8(7)13-2/h3-5,9H,1-2H3
InchiKey:	NYXQGPQZKJJOXJE-UHFFFAOYSA-N
Formula:	C8H10N2O3
SMILES:	CNc1cc([N+](=O)[O-])ccc1OC
Mol. weight [g/mol]:	182.18

Physical Properties

Property code	Value	Unit	Source
gf	129.57	kJ/mol	Joback Method
hf	-84.37	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	62.44	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.645		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1592.30		NIST Webbook
tb	643.51	K	Joback Method
tc	883.07	K	Joback Method
tf	449.88	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.58	J/molxK	643.51	Joback Method
cpg	343.32	J/molxK	683.44	Joback Method
cpg	354.26	J/molxK	723.36	Joback Method
cpg	364.41	J/molxK	763.29	Joback Method
cpg	373.79	J/molxK	803.22	Joback Method
cpg	382.39	J/molxK	843.15	Joback Method
cpg	390.25	J/molxK	883.07	Joback Method

Sources

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=U333466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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