2-Amino-4-nitrophenol, N,N-dimethyl-, methyl ether

Other names: 2-Dimethylamino-4-nitroanisole, methyl ether
Inchi: InChI=1S/C9H12N2O3/c1-10(2)8-6-7(11(12)13)4-5-9(8)14-3/h4-6H,1-3H3
InchiKey: PYIGIQPGDKQYJC-UHFFFAOYSA-N
Formula: C9H12N2O3
SMILES: COc1ccc([N+](=O)[O-])cc1N(C)C
Mol. weight [g/mol]: 196.20

Physical Properties

Property code	Value	Unit	Source
gf	159.38	kJ/mol	Joback Method
hf	-90.95	kJ/mol	Joback Method
hfus	27.90	kJ/mol	Joback Method
hvap	60.27	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.669		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1736.20		NIST Webbook
rinpol	1736.20		NIST Webbook
tb	628.66	K	Joback Method
tc	861.65	K	Joback Method
tf	440.96	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.18	J/mol×K	628.66	Joback Method
cpg	382.39	J/mol×K	667.49	Joback Method
cpg	394.71	J/mol×K	706.32	Joback Method
cpg	406.17	J/mol×K	745.15	Joback Method
cpg	416.79	J/mol×K	783.98	Joback Method
cpg	426.60	J/mol×K	822.81	Joback Method
cpg	435.63	J/mol×K	861.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333468&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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