p-Anisidine, 3-nitro-

Other names: Benzenamine, 4-methoxy-3-nitro-
4-Methoxy-3-nitroaniline
Inchi: InChI=1S/C7H8N2O3/c1-12-7-3-2-5(8)4-6(7)9(10)11/h2-4H,8H2,1H3
InchiKey: RUFOHZDEBFYQSV-UHFFFAOYSA-N
Formula: C7H8N2O3
SMILES: COc1ccc(N)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 168.15
CAS: 577-72-0

Physical Properties

Property code	Value	Unit	Source
gf	98.21	kJ/mol	Joback Method
hf	-83.41	kJ/mol	Joback Method
hfus	24.89	kJ/mol	Joback Method
hvap	64.42	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.186		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	642.99	K	Joback Method
tc	896.92	K	Joback Method
tf	469.21	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.35	J/mol×K	642.99	Joback Method
cpg	301.87	J/mol×K	685.31	Joback Method
cpg	311.62	J/mol×K	727.63	Joback Method
cpg	320.60	J/mol×K	769.95	Joback Method
cpg	328.83	J/mol×K	812.28	Joback Method
cpg	336.32	J/mol×K	854.60	Joback Method
cpg	343.08	J/mol×K	896.92	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=C577720&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume