4-nitro-o-toluidine

Other names:	2-methyl-4-nitroaniline
	5-Nitro-2-aminotoluene
	aniline, 2-methyl-4-nitro-
Inchi:	InChI=1S/C7H8N2O2/c1-5-4-6(9(10)11)2-3-7(5)8/h2-4H,8H2,1H3
InchiKey:	XTTIQGSLJBWVIV-UHFFFAOYSA-N
Formula:	C7H8N2O2
SMILES:	Cc1cc([N+](=O)[O-])ccc1N
Mol. weight [g/mol]:	152.15
CAS:	99-52-5

Physical Properties

Property code	Value	Unit	Source
gf	203.21	kJ/mol	Joback Method
hf	48.81	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.485		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
tb	620.57	K	Joback Method
tc	879.01	K	Joback Method
tf	446.98	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.89	J/mol×K	835.94	Joback Method
cpg	269.53	J/mol×K	620.57	Joback Method
cpg	280.15	J/mol×K	663.64	Joback Method
cpg	289.96	J/mol×K	706.72	Joback Method
cpg	299.00	J/mol×K	749.79	Joback Method
cpg	307.29	J/mol×K	792.87	Joback Method

cpg	321.82	J/mol×K	879.01	Joback Method
cps	217.10	J/mol×K	323.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility and solution thermodynamics of 2-methyl-4-nitroaniline in eleven organic solvents at elevated temperatures:	https://www.doi.org/10.1016/j.jct.2016.10.037
Solubility and preferential solvation of 2-methyl-4-nitroaniline in mixed ethyl acetate + (methanol, ethanol, n-propanol and isopropanol):	https://www.doi.org/10.1016/j.jct.2017.05.044
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=C99525&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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