3-NITRO-O-TOLUIDINE

Other names:	2-Amino-6-nitrotoluene
	2-Methy-3-nitroaniline
	2-Nitro-6-amino toluene
	2-methyl-3-nitroaniline
	Benzenamine, 2-methyl-3-nitro-
	o-Toluidine, 3-nitro-
Inchi:	InChI=1S/C7H8N2O2/c1-5-6(8)3-2-4-7(5)9(10)11/h2-4H,8H2,1H3
InchiKey:	HFCFJYRLBAANKN-UHFFFAOYSA-N
Formula:	C7H8N2O2
SMILES:	Cc1c(N)cccc1[N+](=O)[O-]
Mol. weight [g/mol]:	152.15
CAS:	603-83-8

Physical Properties

Property code	Value	Unit	Source
hf	33.57	kJ/mol	Cheméo Relay (1.0)
hfus	23.71	kJ/mol	Joback Method
hvap	73.84	kJ/mol	Cheméo Relay (1.0)
ie	8.34	eV	Cheméo Relay (1.0)
log10ws	-2.20		Cheméo Relay (1.0)
logp	1.485		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
tb	578.20	K	NIST Webbook
tf	373.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	314.89	J/mol×K	835.94	Joback Method

cpg	321.82	J/mol×K	879.01	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51624e+01
Coeff. B	-5.02238e+03
Coeff. C	-1.01876e+02
Temperature range (K), min.	439.52
Temperature range (K), max.	611.72

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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603838&Units=SI
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
pvap:	Vapor pressure

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point