2-Methyl-5-nitroaniline

Other names:

(2-Methyl-5-nitrophenyl)amine
1-Methyl-2-amino-4-nitrobenzene
2-Amino-4-nitrotoluene
2-Methyl-5-nitro-benzeneamine
2-Methyl-5-nitrobenzenamine
3-Nitro-6-methylaniline
4-Nitro-2-aminotoluene
5-Nitro-O-toluidine
6-Methyl-3-nitroaniline
Amarthol Fast Scarlet G Base
Amarthol Fast Scarlet G Salt
Azoene Fast Scarlet G Salt
Azoene fast scarlet gc base
Azoene fast scarlet gc salt
Azofix scarlet g salt
Azogene fast scarlet g
Azoic diazo component 12, base
C.I. 37105
C.I. Azoic diazo component 12
Conazoic Diazo AB
Dainichi Fast Scarlet G Base
Daito scarlet base g
Devol scarlet b
Devol scarlet g salt
Diabase scarlet g
Diazo fast scarlet g
Fast Scarlet M 4NT Base
Fast red sg base
Fast scarlet base G
Fast scarlet base j
Fast scarlet g
Fast scarlet g base
Fast scarlet g salt
Fast scarlet gc base
Fast scarlet j salt
Fast scarlet t base
Hiltonil fast scarlet g base
Hiltonil fast scarlet g salt
Hiltonil fast scarlet gc base
Kayaku scarlet g base

Lake scarlet g base
Lithosol orange R base
Mitsui scarlet g base
NCI-C01843
Naphthanil scarlet g base
Naphtoelan fast scarlet g base
Naphtoelan fast scarlet g salt
PNOT
RCRA waste number U181
Scarlet base NSP
Scarlet base ciba II
Scarlet base irga II
Scarlet g base
Sugai fast scarlet g base
Symulon scarlet g base
o-Toluidine, 5-nitro-

Inchi: InChI=1S/C7H8N2O2/c1-5-2-3-6(9(10)11)4-7(5)8/h2-4H,8H2,1H3
InchiKey: DSBIJCMXAIKKKI-UHFFFAOYSA-N
Formula: C7H8N2O2
SMILES: Cc1ccc([N+](=O)[O-])cc1N
Mol. weight [g/mol]: 152.15
CAS: 99-55-8

Physical Properties

Property code	Value	Unit	Source
hf	35.72	kJ/mol	Cheméo Relay (1.0)
hfus	23.71	kJ/mol	Joback Method
hvap	76.73	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-2.42		Cheméo Relay (1.0)
logp	1.485		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
tb	559.56	K	Cheméo Relay (1.0)
tf	389.94	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	1.25107e+01
Coeff. B	-3.79209e+03
Coeff. C	-8.72810e+01
Temperature range (K), min.	397.52
Temperature range (K), max.	614.02

Sources

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=C99558&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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