

Benzenamine, 2-methyl-5-nitro-

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-nitroaniline
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: DSBIJCMXAIIKKKI-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
chs	-3809.30 ± 1.30	kJ/mol	NIST Webbook
chs	-3811.70 ± 1.40	kJ/mol	NIST Webbook
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
rinpola	272.14		NIST Webbook
rinpola	272.81		NIST Webbook
tb	620.57	K	Joback Method
tc	879.01	K	Joback Method

tf	446.98	K	Joback Method
vc	0.430	m ³ /kmol	Joback Method

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	$\ln(P_{vp}) = A + B/(T + C)$
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

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C99558&Units=SI>

Legend

chs:	Standard solid enthalpy of combustion
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
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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