

Benzenamine, 4-methyl-3-nitro-

Other names:	1-Amino-3-nitro-4-methylbenzene 2-Nitro-4-aminotoluene 3-Nitro-4-methylaniline 3-Nitro-4-toluidine 3-Nitro-p-toluidine 4-Amino-2-nitrotoluene 4-Methyl-3-nitroaniline 5-Nitro-4-toluidine GI-Amin NSC 7731 m-Nitro-p-toluidine p-Toluidine, 3-nitro-
Inchi:	InChI=1S/C7H8N2O2/c1-5-2-3-6(8)4-7(5)9(10)11/h2-4H,8H2,1H3
InchiKey:	GDIIPKWHAQGCJF-UHFFFAOYSA-N
Formula:	C7H8N2O2
SMILES:	Cc1ccc(N)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	152.15
CAS:	119-32-4

Physical Properties

Property code	Value	Unit	Source
chs	-3828.90 ± 0.50	kJ/mol	NIST Webbook
chs	-3831.30 ± 0.50	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
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	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

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=C119324&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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