1,3-Benzenediamine, 5-nitro-

Other names:	m-Phenylenediamine, 5-nitro-
	1-Nitro-3,5-diaminobenzene
	1,3-Diamino-5-nitrobenzene
	3,5-Diaminonitrobenzene
	5-Nitro-1,3-benzenediamine
	5-nitrobenzene-1,3-diamine
Inchi:	InChI=1S/C6H7N3O2/c7-4-1-5(8)3-6(2-4)9(10)11/h1-3H,7-8H2
InchiKey:	DFWXYHZQNLIBLY-UHFFFAOYSA-N
Formula:	C6H7N3O2
SMILES:	Nc1cc(N)cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	153.14
CAS:	5042-55-7

Physical Properties

Property code	Value	Unit	Source
gf	261.24	kJ/mol	Joback Method
hf	103.24	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	70.42	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.759		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	5351.35	kPa	Joback Method
tb	670.22	K	Joback Method
tc	940.43	K	Joback Method
tf	518.97	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.57	J/mol×K	670.22	Joback Method
cpg	280.82	J/mol×K	715.26	Joback Method
cpg	289.27	J/mol×K	760.29	Joback Method

cpg	296.95	J/mol×K	805.33	Joback Method
cpg	303.92	J/mol×K	850.36	Joback Method
cpg	310.21	J/mol×K	895.40	Joback Method
cpg	315.86	J/mol×K	940.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5042557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

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

Latest version available from:
https://www.chemeo.com/cid/35-233-4/1-3-Benzenediamine-5-nitro.pdf
Generated by Cheméo on 2024-04-29 07:37:06.957091477 +0000 UTC m=+16665475.877668788.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.