

Benzene, 2,4-dimethyl-1-nitro-

Other names:	1,3-Dimethyl-4-nitrobenzene 1-Nitro-2,4-dimethylbenzene 2,4-Dimethyl-1-nitrobenzene 2,4-Dimethylnitrobenzene 4-Nitro-1,3-dimethylbenzene 4-Nitro-1,3-xylene 4-Nitro-m-xylene NSC 50661 benzene, 1,3-dimethyl-4-nitro- m-Xylene, 4-nitro-
Inchi:	InChI=1S/C8H9NO2/c1-6-3-4-8(9(10)11)7(2)5-6/h3-5H,1-2H3
InchiKey:	BBUPBICWUURTNP-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	Cc1ccc([N+](=O)[O-])c(C)c1
Mol. weight [g/mol]:	151.16
CAS:	89-87-2

Physical Properties

Property code	Value	Unit	Source
affp	831.00	kJ/mol	NIST Webbook
basg	798.50	kJ/mol	NIST Webbook
ea	0.88 ± 0.05	eV	NIST Webbook
gf	145.18	kJ/mol	Joback Method
hf	-5.62	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	53.59	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
ie	9.36	eV	NIST Webbook
ie	9.38 ± 0.01	eV	NIST Webbook
log10ws	-3.07		Crippen Method
logp	2.212		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	517.20	K	NIST Webbook
tc	816.66	K	Joback Method
tf	282.68 ± 0.30	K	NIST Webbook
tf	282.76 ± 0.20	K	NIST Webbook

vc	0.458	m3/kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.31	J/mol×K	570.92	Joback Method
cpg	276.23	J/mol×K	611.88	Joback Method
cpg	287.35	J/mol×K	652.83	Joback Method
cpg	297.69	J/mol×K	693.79	Joback Method
cpg	307.28	J/mol×K	734.75	Joback Method
cpg	316.17	J/mol×K	775.71	Joback Method
cpg	324.37	J/mol×K	816.66	Joback Method
hvapt	56.70	kJ/mol	443.00	NIST Webbook
hvapt	57.30	kJ/mol	427.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52259e+01
Coeff. B	-4.57663e+03
Coeff. C	-8.57520e+01
Temperature range (K), min.	392.12
Temperature range (K), max.	547.36

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89872&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous-Methanolic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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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