

4-NITRO-O-XYLENE

Other names:	1,2-Dimethyl-4-nitrobenzene 3,4-Dimethyl-1-nitrobenzene 3,4-Dimethylnitrobenzene 4-Nitro-1,2-dimethylbenzene o-Xylene, 4-nitro- p-Nitro-o-xylene para-Nitro-ortho-xylene
Inchi:	InChI=1S/C8H9NO2/c1-6-3-4-8(9(10)11)5-7(6)2/h3-5H,1-2H3
InchiKey:	HFZKOYWDLDYELC-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	Cc1ccc([N+](=O)[O-])cc1C
Mol. weight [g/mol]:	151.17
CAS:	99-51-4

Physical Properties

Property code	Value	Unit	Source
af	0.5143		Cheméo Relay (1.0)
gf	145.18	kJ/mol	Joback Method
hf	3.91	kJ/mol	Cheméo Relay (1.0)
hfus	21.10	kJ/mol	Joback Method
hvap	68.55	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-3.02		Cheméo Relay (1.0)
logp	2.212		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	522.25	K	Cheméo Relay (1.0)
tc	763.44	K	Cheméo Relay (1.0)
tf	337.34	K	Cheméo Relay (1.0)
vc	0.414	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56588e+01
Coeff. B	-4.74134e+03
Coeff. C	-8.68640e+01
Temperature range (K), min.	395.32
Temperature range (K), max.	545.08

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C99514&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>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
hvac:	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
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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