Benzene, 1,2-dimethoxy-4-nitro-

Other names:	3,4-Dimethoxynitrobenzene
	1,2-Dimethoxy-4-nitrobenzene
	4-Nitroveratrole
	4-Nitrcveratrole
	2-Methoxy-5-nitrophenol, methyl ether
Inchi:	InChI=1S/C8H9NO4/c1-12-7-4-3-6(9(10)11)5-8(7)13-2/h3-5H,1-2H3
InchiKey:	YFWBUVZWCBFSQN-UHFFFAOYSA-N
Formula:	C8H9NO4
SMILES:	COc1ccc([N+](=O)[O-])cc1OC
Mol. weight [g/mol]:	183.16
CAS:	709-09-1

Physical Properties

Property code	Value	Unit	Source
gf	-64.82	kJ/mol	Joback Method
hf	-270.06	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	58.41	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.612		Crippen Method
mcvol	128.980	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1624.10		NIST Webbook
tb	615.76	K	Joback Method
tc	854.02	K	Joback Method
tf	419.45	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.07	J/mol×K	615.76	Joback Method
cpg	320.70	J/mol×K	655.47	Joback Method
cpg	331.62	J/mol×K	695.18	Joback Method

cpg	341.82	J/mol×K	734.89	Joback Method
cpg	351.29	J/mol×K	774.60	Joback Method
cpg	360.02	J/mol×K	814.31	Joback Method
cpg	368.00	J/mol×K	854.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	503.20	K	2.30	NIST Webbook

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=C709091&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume