Benzene, 1-methoxy-2,4-dinitro-

Other names:	1-Methoxy-2,4-dinitrobenzene
	2,4-Dinitro-1-methoxy-benzene
	2,4-Dinitroanisol
	2,4-Dinitroanisole
	2,4-Dinitrophenyl methyl ether
	2,4-Nitroanisole
	Anisole, 2,4-dinitro-
	Dinitroanisole
	NSC 8733
	«alpha»-Dinitroanisole
	Â«alphaÂ»-Dinitroanisole
Inchi:	InChI=1S/C7H6N2O5/c1-14-7-3-2-5(8(10)11)4-6(7)9(12)13/h2-4H,1H3
InchiKey:	CVYZVNVPQRKDLW-UHFFFAOYSA-N
Formula:	C7H6N2O5
SMILES:	COc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	198.13
CAS:	119-27-7

Physical Properties

Property code	Value	Unit	Source
chs	-3425.40 ± 3.40	kJ/mol	NIST Webbook
chs	-3425.40 ± 3.40	kJ/mol	NIST Webbook
gf	67.31	kJ/mol	Joback Method
hf	-127.96	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	70.37	kJ/mol	Joback Method
ie	9.30	eV	NIST Webbook
log10ws	-2.89		Crippen Method
logp	1.512		Crippen Method
mcvol	126.440	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	722.30	K	Joback Method
tc	991.11	K	Joback Method
tf	359.90 ± 1.50	K	NIST Webbook
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.54	J/mol×K	722.30	Joback Method
cpg	331.13	J/mol×K	767.10	Joback Method
cpg	339.81	J/mol×K	811.90	Joback Method
cpg	347.61	J/mol×K	856.71	Joback Method
cpg	354.55	J/mol×K	901.51	Joback Method
cpg	360.63	J/mol×K	946.31	Joback Method
cpg	365.88	J/mol×K	991.11	Joback Method

Sources

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=C119277&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical Properties of an Insensitive Munitions Compound, 2,4-Dinitroanisole:	https://www.doi.org/10.1021/je7006764

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
ie:	Ionization energy
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

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