Benzene, 2-chloro-1-methoxy-4-nitro-

Other names:	Anisole, 2-chloro-4-nitro-
	2-Chloro-4-nitro-anisole
	Orthochloroparanitroanisole
	OCNA
	3-Chloro-4-methoxynitrobenzene
	2-Chloro-1-methoxy-4-nitrobenzene
Inchi:	InChI=1S/C7H6ClNO3/c1-12-7-3-2-5(9(10)11)4-6(7)8/h2-4H,1H3
InchiKey:	DLJPNXLHWMRQIQ-UHFFFAOYSA-N
Formula:	C7H6ClNO3
SMILES:	COc1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]:	187.58
CAS:	4920-79-0

Physical Properties

Property code	Value	Unit	Source
gf	19.83	kJ/mol	Joback Method
hf	-132.94	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	58.16	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.257		Crippen Method
mcvol	121.260	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	607.89	K	Joback Method
tc	858.64	K	Joback Method
tf	415.87	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.98	J/mol×K	607.89	Joback Method
cpg	272.83	J/mol×K	649.68	Joback Method
cpg	281.97	J/mol×K	691.47	Joback Method

cpg	290.43	J/mol×K	733.26	Joback Method
cpg	298.21	J/mol×K	775.05	Joback Method
cpg	305.32	J/mol×K	816.84	Joback Method
cpg	311.78	J/mol×K	858.64	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=C4920790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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