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

Other names:	Anisole, 4-methyl-3-nitro-
	4-Methoxy-2-nitrotoluene
	4-Methyl-3-nitroanisole
	2-Nitro-4-methoxytoluene
Inchi:	InChI=1S/C8H9NO3/c1-6-3-4-7(12-2)5-8(6)9(10)11/h3-5H,1-2H3
InchiKey:	JBORNNNGTJSTLC-UHFFFAOYSA-N
Formula:	C8H9NO3
SMILES:	COc1ccc(C)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	167.16
CAS:	17484-36-5

Physical Properties

Property code	Value	Unit	Source
gf	40.18	kJ/mol	Joback Method
hf	-137.84	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	56.00	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	1.912		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	539.70	K	NIST Webbook
tc	835.30	K	Joback Method
tf	397.22	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.57	J/mol×K	593.34	Joback Method
cpg	298.32	J/mol×K	633.67	Joback Method
cpg	309.33	J/mol×K	673.99	Joback Method
cpg	319.61	J/mol×K	714.32	Joback Method
cpg	329.15	J/mol×K	754.64	Joback Method

cpg	337.99	J/mol×K	794.97	Joback Method
cpg	346.11	J/mol×K	835.30	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=C17484365&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