Naphthalene, 1-methoxy-4-nitro-

Other names:	1-Methoxy-4-nitronaphthalene
	1-Nitro-4-methoxynaphthalene
	methyl 4-nitronaphthyl ether
Inchi:	InChI=1S/C11H9NO3/c1-15-11-7-6-10(12(13)14)8-4-2-3-5-9(8)11/h2-7H,1H3
InchiKey:	YFJKGPRYPHFGQD-UHFFFAOYSA-N
Formula:	C11H9NO3
SMILES:	COc1ccc([N+](=O)[O-])c2ccccc12
Mol. weight [g/mol]:	203.19
CAS:	4900-63-4

Physical Properties

Property code	Value	Unit	Source
ea	1.10 ± 0.10	eV	NIST Webbook
gf	172.09	kJ/mol	Joback Method
hf	-8.69	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	64.32	kJ/mol	Joback Method
log10ws	-4.36		Aqueous Solubility Prediction Method
logp	2.757		Crippen Method
mcvol	145.920	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	680.96	K	Joback Method
tc	938.09	K	Joback Method
tf	463.73	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.34	J/mol×K	680.96	Joback Method
cpg	378.50	J/mol×K	723.81	Joback Method
cpg	389.69	J/mol×K	766.67	Joback Method
cpg	399.95	J/mol×K	809.52	Joback Method

cpg	409.36	J/mol×K	852.38	Joback Method
cpg	417.98	J/mol×K	895.23	Joback Method
cpg	425.89	J/mol×K	938.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4900634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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

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