Phenol, 4-methoxy-2-nitro-

Other names: 4-Methoxy-2-nitrophenol
Inchi: InChI=1S/C7H7NO4/c1-12-5-2-3-7(9)6(4-5)8(10)11/h2-4,9H,1H3
InchiKey: YBUGOACXDPDUIR-UHFFFAOYSA-N
Formula: C7H7NO4
SMILES: COc1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 169.13
CAS: 1568-70-3

Physical Properties

Property code	Value	Unit	Source
gf	-113.23	kJ/mol	Joback Method
hf	-283.04	kJ/mol	Joback Method
hfus	25.87	kJ/mol	Joback Method
hsub	90.80 ± 1.70	kJ/mol	NIST Webbook
hvap	66.13	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.309		Crippen Method
mcvol	114.890	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	646.10	K	Joback Method
tc	901.50	K	Joback Method
tf	485.15	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.65	J/mol×K	858.93	Joback Method
cpg	283.54	J/mol×K	646.10	Joback Method
cpg	292.99	J/mol×K	688.67	Joback Method
cpg	301.75	J/mol×K	731.23	Joback Method
cpg	309.89	J/mol×K	773.80	Joback Method
cpg	317.50	J/mol×K	816.36	Joback Method
cpg	331.41	J/mol×K	901.50	Joback Method

hfust	22.42	kJ/mol	352.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1568703&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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