4'-Methoxy-3'-nitroacetophenone

Other names:	3-Nitro-4-methoxyacetophenone
	4-Methoxy-3-nitroacetophenone
	Ethanone, 1-(4-methoxy-3-nitrophenyl)-
	1-(4-methoxy-3-nitrophenyl)ethan-1-one
Inchi:	InChI=1S/C9H9NO4/c1-6(11)7-3-4-9(14-2)8(5-7)10(12)13/h3-5H,1-2H3
InchiKey:	VXLKYQQBEPCMJE-UHFFFAOYSA-N
Formula:	C9H9NO4
SMILES:	COc1ccc(C(C)=O)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	195.17
CAS:	6277-38-9

Physical Properties

Property code	Value	Unit	Source
gf	-80.32	kJ/mol	Joback Method
hf	-271.06	kJ/mol	Joback Method
hfus	26.48	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	1.806		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	670.09	K	Joback Method
tc	913.32	K	Joback Method
tf	458.42	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.48	J/mol×K	670.09	Joback Method
cpg	355.76	J/mol×K	710.63	Joback Method
cpg	366.20	J/mol×K	751.17	Joback Method
cpg	375.83	J/mol×K	791.70	Joback Method
cpg	384.65	J/mol×K	832.24	Joback Method

cpg	392.67	J/mol×K	872.78	Joback Method
cpg	399.91	J/mol×K	913.32	Joback Method

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=C6277389&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
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