4-Nitrophenyl formate

Other names:	p-Nitrophenyl formate
	Formic acid, 4-nitrophenyl ester
	Formic acid, p-nitrophenyl ester
Inchi:	InChI=1S/C7H5NO4/c9-5-12-7-3-1-6(2-4-7)8(10)11/h1-5H
InchiKey:	IEXRKQFZXJSHOB-UHFFFAOYSA-N
Formula:	C7H5NO4
SMILES:	O=COc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	167.12
CAS:	1865-01-6

Physical Properties

Property code	Value	Unit	Source
gf	-58.13	kJ/mol	Joback Method
hf	-191.31	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.130		Crippen Method
mcvol	110.590	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
tb	614.14	K	Joback Method
tc	861.74	K	Joback Method
tf	415.43	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.65	J/mol×K	614.14	Joback Method
cpg	263.00	J/mol×K	655.41	Joback Method
cpg	271.63	J/mol×K	696.67	Joback Method
cpg	279.56	J/mol×K	737.94	Joback Method
cpg	286.80	J/mol×K	779.21	Joback Method
cpg	293.36	J/mol×K	820.48	Joback Method

cpg	299.26	J/mol×K	861.74	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=C1865016&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