Ethyl 4-nitrobenzoylformate

Inchi: InChI=1S/C10H9NO5/c1-2-16-10(13)9(12)7-3-5-8(6-4-7)11(14)15/h3-6H,2H2,1H3
InchiKey: ZFCXKZCKJZFZGR-UHFFFAOYSA-N
Formula: C10H9NO5
SMILES: CCOC(=O)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 223.18
CAS: 70091-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-191.19	kJ/mol	Joback Method
hf	-392.81	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	73.29	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.341		Crippen Method
mcvol	154.430	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
tb	741.86	K	Joback Method
tc	984.55	K	Joback Method
tf	507.10	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.65	J/mol×K	741.86	Joback Method
cpg	415.18	J/mol×K	782.31	Joback Method
cpg	424.79	J/mol×K	822.76	Joback Method
cpg	433.48	J/mol×K	863.20	Joback Method
cpg	441.29	J/mol×K	903.65	Joback Method
cpg	448.23	J/mol×K	944.10	Joback Method
cpg	454.33	J/mol×K	984.55	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=C70091757&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