1-(4-Nitrophenyl)-1-butanone

Inchi: InChI=1S/C10H11NO3/c1-2-3-10(12)8-4-6-9(7-5-8)11(13)14/h4-7H,2-3H2,1H3
InchiKey: YKLQCIOTHMYXQG-UHFFFAOYSA-N
Formula: C10H11NO3
SMILES: CCCC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 193.20
CAS: 3769-94-6

Physical Properties

Property code	Value	Unit	Source
gf	42.73	kJ/mol	Joback Method
hf	-148.01	kJ/mol	Joback Method
hfus	28.27	kJ/mol	Joback Method
hvap	64.13	kJ/mol	Joback Method
ie	9.90 ± 0.20	eV	NIST Webbook
log10ws	-3.62		Crippen Method
logp	2.578		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	665.57	K	Joback Method
tc	906.59	K	Joback Method
tf	434.94	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.38	J/mol×K	665.57	Joback Method
cpg	383.78	J/mol×K	705.74	Joback Method
cpg	395.25	J/mol×K	745.91	Joback Method
cpg	405.82	J/mol×K	786.08	Joback Method
cpg	415.53	J/mol×K	826.25	Joback Method
cpg	424.45	J/mol×K	866.42	Joback Method
cpg	432.61	J/mol×K	906.59	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=C3769946&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
ie:	Ionization energy
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