4-Nitrophenylacetone

Other names: 2-Propanone, 1-(4-nitrophenyl)-
Inchi: InChI=1S/C9H9NO3/c1-7(11)6-8-2-4-9(5-3-8)10(12)13/h2-5H,6H2,1H3
InchiKey: GEWWCWZGHNIUBW-UHFFFAOYSA-N
Formula: C9H9NO3
SMILES: CC(=O)Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 179.17
CAS: 5332-96-7

Physical Properties

Property code	Value	Unit	Source
gf	34.31	kJ/mol	Joback Method
hf	-127.37	kJ/mol	Joback Method
hfus	25.68	kJ/mol	Joback Method
hvap	61.90	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	1.726		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
tb	642.69	K	Joback Method
tc	889.01	K	Joback Method
tf	423.67	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.04	J/mol×K	642.69	Joback Method
cpg	334.69	J/mol×K	683.74	Joback Method
cpg	345.44	J/mol×K	724.80	Joback Method
cpg	355.32	J/mol×K	765.85	Joback Method
cpg	364.38	J/mol×K	806.91	Joback Method
cpg	372.66	J/mol×K	847.96	Joback Method
cpg	380.22	J/mol×K	889.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5332967&Units=SI
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

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