4-Nitrophenylglyoxylic acid

Other names: Glyoxylic acid, (4-nitrophenyl)-
Inchi: InChI=1S/C8H5NO5/c10-7(8(11)12)5-1-3-6(4-2-5)9(13)14/h1-4H,(H,11,12)
InchiKey: RREPYIWLDJQENS-UHFFFAOYSA-N
Formula: C8H5NO5
SMILES: O=C(O)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 195.13
CAS: 14922-36-2

Physical Properties

Property code	Value	Unit	Source
gf	-239.85	kJ/mol	Joback Method
hf	-371.54	kJ/mol	Joback Method
hfus	28.78	kJ/mol	Joback Method
hvap	83.10	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	0.862		Crippen Method
mcvol	126.250	ml/mol	McGowan Method
pc	4822.53	kPa	Joback Method
tb	765.86	K	Joback Method
tc	1000.94	K	Joback Method
tf	523.15	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.74	J/mol×K	765.86	Joback Method
cpg	327.74	J/mol×K	805.04	Joback Method
cpg	334.08	J/mol×K	844.22	Joback Method
cpg	339.79	J/mol×K	883.40	Joback Method
cpg	344.91	J/mol×K	922.58	Joback Method
cpg	349.48	J/mol×K	961.76	Joback Method
cpg	353.52	J/mol×K	1000.94	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=C14922362&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