1,2-Propanedione, 1-(p-nitrophenyl)-

Inchi: InChI=1S/C9H7NO4/c1-6(11)9(12)7-2-4-8(5-3-7)10(13)14/h2-5H,1H3
InchiKey: WCQBWJSIZYUMDJ-UHFFFAOYSA-N
Formula: C9H7NO4
SMILES: CC(=O)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 193.16
CAS: 6159-25-7

Physical Properties

Property code	Value	Unit	Source
gf	-94.61	kJ/mol	Joback Method
hf	-239.95	kJ/mol	Joback Method
hfus	27.28	kJ/mol	Joback Method
hvap	68.65	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.366		Crippen Method
mcvol	134.470	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	696.56	K	Joback Method
tc	948.65	K	Joback Method
tf	473.60	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.02	J/mol×K	696.56	Joback Method
cpg	342.09	J/mol×K	738.57	Joback Method
cpg	351.26	J/mol×K	780.59	Joback Method
cpg	359.58	J/mol×K	822.60	Joback Method
cpg	367.10	J/mol×K	864.62	Joback Method
cpg	373.85	J/mol×K	906.63	Joback Method
cpg	379.89	J/mol×K	948.65	Joback Method

Sources

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=C6159257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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