Propan-1-one, 3-nitro-1-phenyl-

Other names: 3-nitro-1-phenylpropan-1-one
Inchi: InChI=1S/C9H9NO3/c11-9(6-7-10(12)13)8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey: PMBFWZPQKKUBSU-UHFFFAOYSA-N
Formula: C9H10NO3
SMILES: O=C(CC[N+](=O)[O-])c1ccccc1
Mol. weight [g/mol]: 180.18
CAS: 62847-52-3

Physical Properties

Property code	Value	Unit	Source
gf	43.94	kJ/mol	Joback Method
hf	-115.90	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	61.24	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	1.536		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	637.71	K	Joback Method
tc	883.10	K	Joback Method
tf	411.15	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.39	J/mol×K	637.71	Joback Method
cpg	336.26	J/mol×K	678.61	Joback Method
cpg	347.17	J/mol×K	719.51	Joback Method
cpg	357.17	J/mol×K	760.40	Joback Method
cpg	366.32	J/mol×K	801.30	Joback Method
cpg	374.66	J/mol×K	842.20	Joback Method
cpg	382.27	J/mol×K	883.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62847523&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