«alpha»-Nitroacetophenone

Other names:	Ethanone, 2-nitro-1-phenyl-
	Benzoylnitromethane
	Acetophenone, 2-nitro-
	«omega»-Nitroacetophenone
	2-Nitro-1-phenylethanone
	2-Nitroacetophenone
	Nitromethyl phenyl ketone
	NSC 4509
Inchi:	InChI=1S/C8H7NO3/c10-8(6-9(11)12)7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	JTWHVBNYYWFXSI-UHFFFAOYSA-N
Formula:	C8H7NO3
SMILES:	O=C(C[N+](=O)[O-])c1ccccc1
Mol. weight [g/mol]:	165.15
CAS:	614-21-1

Physical Properties

Property code	Value	Unit	Source
gf	35.52	kJ/mol	Joback Method
hf	-95.26	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	59.02	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.146		Crippen Method
mcvol	118.810	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	614.83	K	Joback Method
tc	865.79	K	Joback Method
tf	399.88	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.61	J/mol×K	614.83	Joback Method

cpg	288.62	J/mol×K	656.66	Joback Method
cpg	298.72	J/mol×K	698.48	Joback Method
cpg	307.93	J/mol×K	740.31	Joback Method
cpg	316.32	J/mol×K	782.14	Joback Method
cpg	323.95	J/mol×K	823.96	Joback Method
cpg	330.85	J/mol×K	865.79	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=C614211&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