Acetamide, N-(2-nitrophenyl)-

Other names:	2'-Nitroacetanilide
	2-Nitroacetanilide
	Acetanilide, 2'-nitro-
	o-Nitroacetanilide
Inchi:	InChI=1S/C8H8N2O3/c1-6(11)9-7-4-2-3-5-8(7)10(12)13/h2-5H,1H3,(H,9,11)
InchiKey:	BUNFNRVLMKHKIT-UHFFFAOYSA-N
Formula:	C8H8N2O3
SMILES:	CC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	180.16
CAS:	552-32-9

Physical Properties

Property code	Value	Unit	Source
gf	115.28	kJ/mol	Joback Method
hf	-53.26	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	66.11	kJ/mol	Joback Method
ie	8.85	eV	NIST Webbook
log10ws	-1.91		Aqueous Solubility Prediction Method
logp	1.553		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	669.98	K	Joback Method
tc	918.65	K	Joback Method
tf	366.20 ± 0.50	K	NIST Webbook
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.18	J/mol×K	669.98	Joback Method
cpg	330.79	J/mol×K	711.43	Joback Method
cpg	340.52	J/mol×K	752.87	Joback Method

cpg	349.41	J/mol×K	794.32	Joback Method
cpg	357.50	J/mol×K	835.76	Joback Method
cpg	364.84	J/mol×K	877.21	Joback Method
cpg	371.48	J/mol×K	918.65	Joback Method
hvapt	44.00	kJ/mol	533.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C552329&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
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