Benzeneacetic acid, 3-nitro-

Other names:	3-Nitrophenylacetic acid
	m-Nitrophenyl acetic acid
	Acetic acid, (m-nitrophenyl)-
	3-Nitrobenzeneacetic acid
Inchi:	InChI=1S/C8H7NO4/c10-8(11)5-6-2-1-3-7(4-6)9(12)13/h1-4H,5H2,(H,10,11)
InchiKey:	WUKHOVCMWXMOOA-UHFFFAOYSA-N
Formula:	C8H7NO4
SMILES:	O=C(O)Cc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	181.15
CAS:	1877-73-2

Physical Properties

Property code	Value	Unit	Source
gf	-110.93	kJ/mol	Joback Method
hf	-258.96	kJ/mol	Joback Method
hfus	27.18	kJ/mol	Joback Method
hvap	76.36	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.222		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	711.99	K	Joback Method
tc	941.67	K	Joback Method
tf	390.65 ± 2.00	K	NIST Webbook
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.34	J/mol×K	711.99	Joback Method
cpg	324.71	J/mol×K	750.27	Joback Method
cpg	332.40	J/mol×K	788.55	Joback Method
cpg	339.46	J/mol×K	826.83	Joback Method
cpg	345.92	J/mol×K	865.11	Joback Method

cpg	351.81	J/mol×K	903.39	Joback Method
cpg	357.18	J/mol×K	941.67	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=C1877732&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