

Acetamide, N-(3-nitrophenyl)-

Other names:	Acetanilide, 3'-nitro-m-Nitroacetanilide N-(3-Nitrophenyl)acetamide N-Acetyl-m-nitroaniline 3-Nitro-N-acetylaniline 3'-Nitroacetanilide 3-Nitroacetanilide N-(3-Nitrophenyl)acetic acid amide
Inchi:	InChI=1S/C8H8N2O3/c1-6(11)9-7-3-2-4-8(5-7)10(12)13/h2-5H,1H3,(H,9,11)
InchiKey:	KFTYNYHJHKCRKU-UHFFFAOYSA-N
Formula:	C8H8N2O3
SMILES:	CC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	180.16
CAS:	122-28-1

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	8.80 ± 0.20	eV	NIST Webbook
log10ws	-2.33		Crippen 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	427.70 ± 0.50	K	NIST Webbook
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122281&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
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

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