2',4'-Dinitroacetanilide

Other names:	2,4-Dinitroacetanilide
	Acetamide, N-(2,4-dinitrophenyl)-
	Acetanilide, 2',4'-dinitro-
	1-Acetamido-2,4-dinitrobenzene
Inchi:	InChI=1S/C8H7N3O5/c1-5(12)9-7-3-2-6(10(13)14)4-8(7)11(15)16/h2-4H,1H3,(H,9,12)
InchiKey:	BRZYMGKDOVQJGX-UHFFFAOYSA-N
Formula:	C8H7N3O5
SMILES:	CC(=O)Nc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	225.16
CAS:	610-53-7

Physical Properties

Property code	Value	Unit	Source
gf	141.20	kJ/mol	Joback Method
hf	-75.49	kJ/mol	Joback Method
hfus	39.16	kJ/mol	Joback Method
hvap	83.37	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	1.461		Crippen Method
mcvol	146.210	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
tb	826.80	K	Joback Method
tc	1093.23	K	Joback Method
tf	621.19	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.91	J/mol×K	826.80	Joback Method
cpg	406.35	J/mol×K	871.21	Joback Method
cpg	413.86	J/mol×K	915.61	Joback Method
cpg	420.52	J/mol×K	960.02	Joback Method
cpg	426.37	J/mol×K	1004.42	Joback Method

cpg	431.46	J/mol×K	1048.83	Joback Method
cpg	435.85	J/mol×K	1093.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C610537&Units=SI

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