

# 2,4-Dimethyl-6-nitro acetanilide

<b>Inchi:</b>	InChI=1S/C10H12N2O3/c1-6-4-7(2)10(11-8(3)13)9(5-6)12(14)15/h4-5H,1-3H3,(H,11,13)
<b>InchiKey:</b>	PXXMBAOADHXJSE-UHFFFAOYSA-N
<b>Formula:</b>	C10H12N2O3
<b>SMILES:</b>	CC(=O)Nc1c(C)cc(C)cc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	208.21
<b>CAS:</b>	606-38-2

## Physical Properties

Property code	Value	Unit	Source
gf	112.86	kJ/mol	Joback Method
hf	-117.48	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	71.89	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.170		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
tb	725.70	K	Joback Method
tc	965.57	K	Joback Method
tf	512.64	K	Joback Method
vc	0.611	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.95	J/molxK	725.70	Joback Method
cpg	427.68	J/molxK	765.68	Joback Method
cpg	438.53	J/molxK	805.66	Joback Method
cpg	448.53	J/molxK	845.63	Joback Method
cpg	457.71	J/molxK	885.61	Joback Method
cpg	466.10	J/molxK	925.59	Joback Method
cpg	473.74	J/molxK	965.57	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C606382&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C606382&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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