

4'-Methyl-2'-nitroacetanilide

Other names:	Acetamide, N-(4-methyl-2-nitrophenyl)- p-Acetotoluidide, 2'-nitro- 2'-Nitro-p-acetotoluidide N-(4-methyl-2-nitrophenyl)acetamide
Inchi:	InChI=1S/C9H10N2O3/c1-6-3-4-8(10-7(2)12)9(5-6)11(13)14/h3-5H,1-2H3,(H,10,12)
InchiKey:	LQZGUJSFLJIJKA-UHFFFAOYSA-N
Formula:	C9H10N2O3
SMILES:	CC(=O)Nc1ccc(C)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	194.19
CAS:	612-45-3

Physical Properties

Property code	Value	Unit	Source
gf	114.07	kJ/mol	Joback Method
hf	-85.37	kJ/mol	Joback Method
hfus	30.39	kJ/mol	Joback Method
hvap	69.00	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.862		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	697.84	K	Joback Method
tc	941.94	K	Joback Method
tf	488.85	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.33	J/molxK	697.84	Joback Method
cpg	378.53	J/molxK	738.52	Joback Method
cpg	388.85	J/molxK	779.21	Joback Method
cpg	398.34	J/molxK	819.89	Joback Method
cpg	407.02	J/molxK	860.58	Joback Method

cpg	414.93	J/mol×K	901.26	Joback Method
cpg	422.12	J/mol×K	941.94	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=C612453&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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