2,4-Dimethyl-6-nitroaniline

Other names: Benzenamine, 2,4-dimethyl-6-nitro-
6-nitro-2,4-xylidine
Inchi: InChI=1S/C8H10N2O2/c1-5-3-6(2)8(9)7(4-5)10(11)12/h3-4H,9H2,1-2H3
InchiKey: VSRYYONYIUUFFY-UHFFFAOYSA-N
Formula: C8H10N2O2
SMILES: Cc1cc(C)c(N)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 166.18
CAS: 1635-84-3

Physical Properties

Property code	Value	Unit	Source
gf	202.00	kJ/mol	Joback Method
hf	16.70	kJ/mol	Joback Method
hfus	25.91	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	1.794		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	648.43	K	Joback Method
tc	901.82	K	Joback Method
tf	470.77	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.69	J/mol×K	648.43	Joback Method
cpg	326.07	J/mol×K	690.66	Joback Method
cpg	336.64	J/mol×K	732.89	Joback Method
cpg	346.43	J/mol×K	775.12	Joback Method
cpg	355.46	J/mol×K	817.36	Joback Method
cpg	363.78	J/mol×K	859.59	Joback Method
cpg	371.40	J/mol×K	901.82	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=C1635843&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