6-Nitroveratraldehyde

Other names:	3,4-Dimethoxy-6-nitrobenzaldehyde
	Benzaldehyde, 4,5-dimethoxy-2-nitro-
Inchi:	InChI=1S/C9H9NO5/c1-14-8-3-6(5-11)7(10(12)13)4-9(8)15-2/h3-5H,1-2H3
InchiKey:	YWSPWKXREVSQCA-UHFFFAOYSA-N
Formula:	C9H9NO5
SMILES:	COc1cc(C=O)c([N+](=O)[O-])cc1OC
Mol. weight [g/mol]:	211.17
CAS:	20357-25-9

Physical Properties

Property code	Value	Unit	Source
gf	-165.55	kJ/mol	Joback Method
hf	-387.75	kJ/mol	Joback Method
hfus	27.97	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.424		Crippen Method
mcvol	144.640	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	692.28	K	Joback Method
tc	927.60	K	Joback Method
tf	485.24	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.96	J/mol×K	692.28	Joback Method
cpg	377.68	J/mol×K	731.50	Joback Method
cpg	387.65	J/mol×K	770.72	Joback Method
cpg	396.85	J/mol×K	809.94	Joback Method
cpg	405.26	J/mol×K	849.16	Joback Method
cpg	412.87	J/mol×K	888.38	Joback Method
cpg	419.67	J/mol×K	927.60	Joback Method

Sources

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=C20357259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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