6-Nitroveratryl alcohol

Other names: 3,4-Dimethoxy-6-nitrobenzyl alcohol
Benzenemethanol, 4,5-dimethoxy-2-nitro-
Inchi: InChI=1S/C9H11NO5/c1-14-8-3-6(5-11)7(10(12)13)4-9(8)15-2/h3-4,11H,5H2,1-2H3
InchiKey: WBSCOJBVYHQOFB-UHFFFAOYSA-N
Formula: C9H11NO5
SMILES: COc1cc(CO)c([N+](=O)[O-])cc1OC
Mol. weight [g/mol]: 213.19
CAS: 1016-58-6

Physical Properties

Property code	Value	Unit	Source
gf	-202.85	kJ/mol	Joback Method
hf	-454.40	kJ/mol	Joback Method
hfus	29.77	kJ/mol	Joback Method
hvap	77.98	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.104		Crippen Method
mcvol	148.940	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	735.80	K	Joback Method
tc	952.44	K	Joback Method
tf	504.06	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.97	J/mol×K	735.80	Joback Method
cpg	410.95	J/mol×K	771.91	Joback Method
cpg	420.24	J/mol×K	808.01	Joback Method
cpg	428.85	J/mol×K	844.12	Joback Method
cpg	436.76	J/mol×K	880.23	Joback Method
cpg	443.97	J/mol×K	916.34	Joback Method
cpg	450.46	J/mol×K	952.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1016586&Units=SI
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

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