1,2-Dimethoxy-4,5-dinitrobenzene

Other names: 4,5-Dinitro veratrole
Inchi: InChI=1S/C8H8N2O6/c1-15-7-3-5(9(11)12)6(10(13)14)4-8(7)16-2/h3-4H,1-2H3
InchiKey: WFDHPWTYKOAFBJ-UHFFFAOYSA-N
Formula: C8H8N2O6
SMILES: COc1cc([N+](=O)[O-])c([N+](=O)[O-])cc1OC
Mol. weight [g/mol]: 228.16
CAS: 3395-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-38.90	kJ/mol	Joback Method
hf	-292.29	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	1.520		Crippen Method
mcvol	146.400	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	772.58	K	Joback Method
tc	1030.98	K	Joback Method
tf	575.58	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.28	J/mol×K	772.58	Joback Method
cpg	402.28	J/mol×K	815.65	Joback Method
cpg	411.30	J/mol×K	858.71	Joback Method
cpg	419.34	J/mol×K	901.78	Joback Method
cpg	426.37	J/mol×K	944.85	Joback Method
cpg	432.37	J/mol×K	987.92	Joback Method
cpg	437.33	J/mol×K	1030.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3395037&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

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