4,5-Dimethoxy-2-nitrotoluene

Inchi: InChI=1S/C9H11NO4/c1-6-4-8(13-2)9(14-3)5-7(6)10(11)12/h4-5H,1-3H3
InchiKey: BNJRARLHTLUQCH-UHFFFAOYSA-N
Formula: C9H11NO4
SMILES: COc1cc(C)c([N+](=O)[O-])cc1OC
Mol. weight [g/mol]: 197.19
CAS: 7509-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-66.03	kJ/mol	Joback Method
hf	-302.17	kJ/mol	Joback Method
hfus	25.68	kJ/mol	Joback Method
hvap	61.30	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	1.920		Crippen Method
mcvol	143.070	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	643.62	K	Joback Method
tc	877.93	K	Joback Method
tf	443.24	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.33	J/mol×K	643.62	Joback Method
cpg	367.65	J/mol×K	682.67	Joback Method
cpg	379.24	J/mol×K	721.72	Joback Method
cpg	390.08	J/mol×K	760.77	Joback Method
cpg	400.16	J/mol×K	799.83	Joback Method
cpg	409.45	J/mol×K	838.88	Joback Method
cpg	417.95	J/mol×K	877.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7509117&Units=SI

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