1-Nitro-2,4,6-trimethoxybenzene

Other names:	Benzene, 1,3,5-trimethoxy-2-nitro- 2,4,6-Trimethoxynitrobenzene
Inchi:	InChI=1S/C9H11NO5/c1-13-6-4-7(14-2)9(10(11)12)8(5-6)15-3/h4-5H,1-3H3
InchiKey:	VWYAWLZEMLQGJH-UHFFFAOYSA-N
Formula:	C9H11NO5
SMILES:	COc1cc(OC)c([N+](=O)[O-])c(OC)c1
Mol. weight [g/mol]:	213.19
CAS:	14227-18-0

Physical Properties

Property code	Value	Unit	Source
gf	-171.03	kJ/mol	Joback Method
hf	-434.39	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	63.71	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.621		Crippen Method
mcvol	148.940	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	666.04	K	Joback Method
tc	896.96	K	Joback Method
tf	465.47	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.95	J/mol×K	666.04	Joback Method
cpg	391.13	J/mol×K	704.53	Joback Method
cpg	402.59	J/mol×K	743.01	Joback Method
cpg	413.27	J/mol×K	781.50	Joback Method
cpg	423.15	J/mol×K	819.99	Joback Method
cpg	432.20	J/mol×K	858.48	Joback Method
cpg	440.37	J/mol×K	896.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14227180&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