Methyl 2,6-dimethoxy-3-nitrobenzoate

Inchi: InChI=1S/C10H11NO6/c1-15-7-5-4-6(11(13)14)9(16-2)8(7)10(12)17-3/h4-5H,1-3H3
InchiKey: HVVQDBFINNUQBK-UHFFFAOYSA-N
Formula: C10H11NO6
SMILES: COC(=O)c1c(OC)ccc([N+](=O)[O-])c1OC
Mol. weight [g/mol]: 241.20
CAS: 55776-20-0

Physical Properties

Property code	Value	Unit	Source
gf	-291.53	kJ/mol	Joback Method
hf	-567.61	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	72.68	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.399		Crippen Method
mcvol	164.600	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
tb	742.79	K	Joback Method
tc	975.03	K	Joback Method
tf	526.67	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.21	J/mol×K	742.79	Joback Method
cpg	451.64	J/mol×K	781.50	Joback Method
cpg	462.17	J/mol×K	820.20	Joback Method
cpg	471.77	J/mol×K	858.91	Joback Method
cpg	480.40	J/mol×K	897.61	Joback Method
cpg	488.04	J/mol×K	936.32	Joback Method
cpg	494.64	J/mol×K	975.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55776200&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