bis-(4-Nitrophenyl)-hydroxyacetic acid, methyl ester

Other names: para,para'-«alpha»-Hydroxydinitrodiphenylacetic acid, methyl ester
Inchi: InChI=1S/C15H12N2O7/c1-24-14(18)15(19,10-2-6-12(7-3-10)16(20)21)11-4-8-13(9-5-11
InchiKey: NLIGJKPJSALUSB-UHFFFAOYSA-N
Formula: C15H12N2O7
SMILES: COC(=O)C(O)(c1ccc([N+](=O)[O-])cc1)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 332.26

Physical Properties

Property code	Value	Unit	Source
gf	-15.82	kJ/mol	Joback Method
hf	-330.11	kJ/mol	Joback Method
hfus	44.09	kJ/mol	Joback Method
hvap	112.58	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	1.912		Crippen Method
mcvol	222.840	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2732.00		NIST Webbook
rinpol	2732.00		NIST Webbook
rinpol	2732.00		NIST Webbook
tb	1074.84	K	Joback Method
tc	1340.57	K	Joback Method
tf	759.31	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.54	J/mol×K	1074.84	Joback Method
cpg	690.24	J/mol×K	1119.13	Joback Method
cpg	696.19	J/mol×K	1163.42	Joback Method
cpg	701.51	J/mol×K	1207.71	Joback Method

cpg	706.32	J/mol×K	1252.00	Joback Method
cpg	710.72	J/mol×K	1296.29	Joback Method
cpg	714.85	J/mol×K	1340.57	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=R190075&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume