Methylglyoxal 2,4-dinitrophenylosazone

Inchi: InChI=1S/C15H12N8O8/c1-9(17-19-13-5-3-11(21(26)27)7-15(13)23(30)31)8-16-18-12-4-
InchiKey: MYLXEBSTNQBXAJ-UHFFFAOYSA-N
Formula: C15H12N8O8
SMILES: CC(C=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-])=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 432.30
CAS: 1107-69-3

Physical Properties

Property code	Value	Unit	Source
chs	-7795.00	kJ/mol	NIST Webbook
hf	292.80	kJ/mol	Joback Method
hfs	160.00	kJ/mol	NIST Webbook
hvap	142.13	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	3.205		Crippen Method
mcvol	275.690	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
tb	1476.82	K	Joback Method
tc	1809.32	K	Joback Method

Sources

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=C1107693&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation 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