2,4,6-Tripicryltriazine

Inchi: InChI=1S/C21H6N12O18/c34-25(35)7-1-10(28(40)41)16(11(2-7)29(42)43)19-22-20(17-1
InchiKey: FBPVIIPYBVZWJZ-UHFFFAOYSA-N
Formula: C21H6N12O18
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(-c2nc(-c3c([N+](=O)[O-])cc([N+](=O)[O-])cc3[N+](=O)[O
Mol. weight [g/mol]: 714.34
CAS: 49753-54-0

Physical Properties

Property code	Value	Unit	Source
chs	-9417.70 ± 7.00	kJ/mol	NIST Webbook
chs	-9439.10 ± 7.10	kJ/mol	NIST Webbook
hfs	296.50 ± 7.00	kJ/mol	NIST Webbook
hfs	318.00 ± 17.00	kJ/mol	NIST Webbook
log10ws	-14.43		Crippen Method
logp	4.046		Crippen Method
mcvol	398.430	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	167.90	kJ/mol	515.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C49753540&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume