2,4,7-Trinitroxanthen-9-one

Other names: 2,4,7-Trinitroxanthone
Inchi: InChI=1S/C13H5N3O8/c17-12-8-3-6(14(18)19)1-2-11(8)24-13-9(12)4-7(15(20)21)5-10(1
InchiKey: GRKGPRVKUQAYIM-UHFFFAOYSA-N
Formula: C13H5N3O8
SMILES: O=c1c2cc([N+](=O)[O-])ccc2oc2c([N+](=O)[O-])cc([N+](=O)[O-])cc12
Mol. weight [g/mol]: 331.19
CAS: 131032-92-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.19		Crippen Method
logp	2.671		Crippen Method
mcvol	195.350	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	31.40	kJ/mol	477.80	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C131032923&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume