2,7-DINITRO-9H-XANTHEN-9-ONE

Other names: 2,7-Dinitroxanthone
Inchi: InChI=1S/C13H6N2O6/c16-13-9-5-7(14(17)18)1-3-11(9)21-12-4-2-8(15(19)20)6-10(12)1
InchiKey: XMSWUZGXFRVEHY-UHFFFAOYSA-N
Formula: C13H6N2O6
SMILES: O=c1c2cc([N+](=O)[O-])ccc2oc2ccc([N+](=O)[O-])cc12
Mol. weight [g/mol]: 286.20

Physical Properties

Property code	Value	Unit	Source
hf	-71.75	kJ/mol	Cheméo Relay (1.0)
hvap	118.29	kJ/mol	Cheméo Relay (1.0)
ie	9.47	eV	Cheméo Relay (1.0)
log10ws	-4.99		Cheméo Relay (1.0)
logp	2.763		Crippen Method
mcvol	177.930	ml/mol	McGowan Method
tb	671.81	K	Cheméo Relay (1.0)
tf	523.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.59	kJ/mol	540.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51792188&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point