

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
CAS:	51792-18-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.54		Crippen Method
logp	2.763		Crippen Method
mccvol	177.930	ml/mol	McGowan Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C51792188&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

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