9H-Fluoren-9-one, 2,4,5,7-tetranitro-

Other names:	Fluoren-9-one, 2,4,5,7-tetranitro-
	2,4,5,7-Tetranitro-9-fluorenone
	2,4,5,7-Tetranitrofluoren-9-one
	2,4,5,7-Tetranitrofluorenone
	Tetranitrofluorenone
	9H-Fluoren-9-one, tetranitro-
	2,4,5,7-Tetranitro-9H-fluoren-9-one
Inchi:	InChI=1S/C13H4N4O9/c18-13-7-1-5(14(19)20)3-9(16(23)24)11(7)12-8(13)2-6(15(21)22)4
InchiKey:	JOERSAVCLPYNIZ-UHFFFAOYSA-N
Formula:	C13H4N4O9
SMILES:	O=C1c2cc([N+](=O)[O-])cc([N+](=O)[O-])c2-c2c1cc([N+](=O)[O-])cc2[N+](=O)[O-]
Mol. weight [g/mol]:	360.19
CAS:	746-53-2

Physical Properties

Property code	Value	Unit	Source
gf	337.89	kJ/mol	Joback Method
hf	17.31	kJ/mol	Joback Method
hfus	61.39	kJ/mol	Joback Method
hvap	123.55	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	2.531		Crippen Method
mcvol	206.900	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	486.49		NIST Webbook
rinpol	486.49		NIST Webbook
tb	1258.13	K	Joback Method
tc	1573.93	K	Joback Method
tf	1036.11	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	626.42	J/mol×K	1258.13	Joback Method
cpg	633.00	J/mol×K	1310.76	Joback Method
cpg	639.58	J/mol×K	1363.40	Joback Method
cpg	646.33	J/mol×K	1416.03	Joback Method
cpg	653.43	J/mol×K	1468.66	Joback Method
cpg	661.04	J/mol×K	1521.30	Joback Method
cpg	669.34	J/mol×K	1573.93	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=C746532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume