9H-Fluoren-9-one, 2,4,7-trinitro-

Other names: 9H-Fluoren-9-one, 2,4,7-trinitro-
Fluoren-9-one, 2,4,7-trinitro-
TNF
2,4,7-Trinitrofluoren-9-one
2,4,7-Trinitro-9-fluorenone
Inchi: InChI=1S/C13H5N3O7/c17-13-9-3-6(14(18)19)1-2-8(9)12-10(13)4-7(15(20)21)5-11(12)1
InchiKey: VHQGURIJMFPBKS-UHFFFAOYSA-N
Formula: C13H5N3O7
SMILES: O=C1c2cc([N+](=O)[O-])ccc2-c2c1cc([N+](=O)[O-])cc2[N+](=O)[O-]
Mol. weight [g/mol]: 315.20

Physical Properties

Property code	Value	Unit	Source
hf	62.45	kJ/mol	Cheméo Relay (1.0)
hfus	50.42	kJ/mol	Joback Method
hvap	119.14	kJ/mol	Cheméo Relay (1.0)
ie	10.15	eV	Cheméo Relay (1.0)
log10ws	-5.09		Cheméo Relay (1.0)
logp	2.623		Crippen Method
mcvol	189.480	ml/mol	McGowan Method
tb	658.93	K	Cheméo Relay (1.0)
tf	449.00 ± 0.30	K	NIST Webbook
tf	449.00 ± 0.50	K	NIST Webbook
tf	448.15 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.97	J/mol×K	1101.31	Joback Method
cpg	569.58	J/mol×K	1151.96	Joback Method
cpg	576.85	J/mol×K	1202.62	Joback Method
cpg	583.94	J/mol×K	1253.27	Joback Method
cpg	591.01	J/mol×K	1303.93	Joback Method
cpg	598.21	J/mol×K	1354.58	Joback Method

cpg	605.71	J/mol×K	1405.24	Joback Method
hfust	23.50	kJ/mol	449.20	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C129793&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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