2,6-Dinitro-9H-fluoren-9-one

Other names: 2,6-dinitro-9-fluorenone
Inchi: InChI=1S/C13H6N2O5/c16-13-10-4-2-7(14(17)18)5-11(10)9-3-1-8(15(19)20)6-12(9)13/h
InchiKey: XHBAHYMCKJTKJV-UHFFFAOYSA-N
Formula: C13H6N2O5
SMILES: O=C1c2cc([N+](=O)[O-])ccc2-c2cc([N+](=O)[O-])ccc21
Mol. weight [g/mol]: 270.20

Physical Properties

Property code	Value	Unit	Source
gf	286.05	kJ/mol	Joback Method
hf	61.77	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	89.04	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	2.714		Crippen Method
mcvol	172.060	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
rinpol	421.88		NIST Webbook
tb	944.49	K	Joback Method
tc	1237.67	K	Joback Method
tf	723.85	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.54	J/mol×K	944.49	Joback Method
cpg	500.72	J/mol×K	993.35	Joback Method
cpg	509.24	J/mol×K	1042.22	Joback Method
cpg	517.25	J/mol×K	1091.08	Joback Method
cpg	524.90	J/mol×K	1139.94	Joback Method
cpg	532.34	J/mol×K	1188.80	Joback Method
cpg	539.71	J/mol×K	1237.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U326028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

Latest version available from:
https://www.chemeo.com/cid/60-023-9/2-6-Dinitro-9H-fluoren-9-one.pdf
Generated by Cheméo on 2024-04-18 16:00:49.963330814 +0000 UTC m=+15745298.883908130.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.