9H-Fluorene, 2-nitro-

Other names:	2-Nitro-9H-fluorene
	2-Nitrofluorene
	Fluorene, 2-nitro-
Inchi:	InChI=1S/C13H9NO2/c15-14(16)11-5-6-13-10(8-11)7-9-3-1-2-4-12(9)13/h1-6,8H,7H2
InchiKey:	XFOHWECQTFIEIX-UHFFFAOYSA-N
Formula:	C13H9NO2
SMILES:	O=[N+]([O-])c1ccc2c(c1)Cc1ccccc1-2
Mol. weight [g/mol]:	211.22
CAS:	607-57-8

Physical Properties

Property code	Value	Unit	Source
gf	382.72	kJ/mol	Joback Method
hf	221.70	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	67.54	kJ/mol	Joback Method
log10ws	-4.72		Aqueous Solubility Prediction Method
logp	3.166		Crippen Method
mcvol	153.070	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	352.22		NIST Webbook
rinpol	352.42		NIST Webbook
rinpol	353.06		NIST Webbook
rinpol	359.10		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	351.77		NIST Webbook
rinpol	350.98		NIST Webbook
rinpol	353.06		NIST Webbook
rinpol	352.17		NIST Webbook
rinpol	352.12		NIST Webbook
rinpol	2066.00		NIST Webbook
rinpol	352.60		NIST Webbook
tb	719.85	K	Joback Method

tc	990.35	K	Joback Method
tf	429.89	K	Experimental and computational study of the thermodynamic properties of 2-nitrofluorene and 2-aminofluorene
tf	429.65	K	Aqueous Solubility Prediction Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.59	J/mol×K	719.85	Joback Method
cpg	408.63	J/mol×K	764.93	Joback Method
cpg	419.68	J/mol×K	810.02	Joback Method
cpg	429.94	J/mol×K	855.10	Joback Method
cpg	439.57	J/mol×K	900.18	Joback Method
cpg	448.76	J/mol×K	945.26	Joback Method
cpg	457.69	J/mol×K	990.35	Joback Method
hsubt	114.20 ± 3.00	kJ/mol	366.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C607578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental and computational study of the thermodynamic properties of 2-nitrofluorene and 2-aminofluorene:	https://www.doi.org/10.1016/j.jct.2014.03.005

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

hsubt:	Enthalpy of sublimation at a given temperature
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