9H-Fluoren-9-one, 3-nitro-

Other names:	3-Nitrofluorenone
	3-Nitro-9-fluorenone
	9-Fluorenone, 3-nitro
	3-nitrofluoren-9-one
Inchi:	InChI=1S/C13H7NO3/c15-13-10-4-2-1-3-9(10)12-7-8(14(16)17)5-6-11(12)13/h1-7H
InchiKey:	GLVSVKSIYXDZHY-UHFFFAOYSA-N
Formula:	C13H7NO3
SMILES:	O=C1c2ccccc2-c2cc([N+](=O)[O-])ccc21
Mol. weight [g/mol]:	225.20
CAS:	42135-22-8

Physical Properties

Property code	Value	Unit	Source
gf	260.13	kJ/mol	Joback Method
hf	84.00	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	71.79	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	2.806		Crippen Method
mcvol	154.640	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	363.40		NIST Webbook
rinpol	363.40		NIST Webbook
rinpol	355.07		NIST Webbook
rinpol	355.53		NIST Webbook
rinpol	355.07		NIST Webbook
tb	787.67	K	Joback Method
tc	1067.93	K	Joback Method
tf	567.72	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	414.34	J/mol×K	787.67	Joback Method
cpg	425.55	J/mol×K	834.38	Joback Method
cpg	435.83	J/mol×K	881.09	Joback Method
cpg	445.32	J/mol×K	927.80	Joback Method
cpg	454.14	J/mol×K	974.51	Joback Method
cpg	462.43	J/mol×K	1021.22	Joback Method
cpg	470.32	J/mol×K	1067.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42135228&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

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