2-Nitro-9-fluorenone

Other names: 9H-Fluoren-9-one, 2-nitro-
9-Fluorenone, 2-nitro
Inchi: InChI=1S/C13H7NO3/c15-13-11-4-2-1-3-9(11)10-6-5-8(14(16)17)7-12(10)13/h1-7H
InchiKey: AJEAHBZZHSLIQP-UHFFFAOYSA-N
Formula: C13H7NO3
SMILES: O=C1c2ccccc2-c2ccc([N+](=O)[O-])cc21
Mol. weight [g/mol]: 225.20
CAS: 3096-52-4

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	366.83		NIST Webbook
rinpol	366.80		NIST Webbook
rinpol	364.70		NIST Webbook
rinpol	366.80		NIST Webbook
rinpol	364.70		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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3096524&Units=SI

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