2-Nitrofluorene-d9

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/i1D
InchiKey: XFOHWECQTFIEIX-MFNUZUOVSA-N
Formula: C13D9NO2
SMILES: O=[N+]([O-])c1ccc2c(c1)Cc1ccccc1-2
Mol. weight [g/mol]: 220.27

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	-5.07		Crippen Method
logp	3.166		Crippen Method
mcvol	153.070	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	350.07		NIST Webbook
rinpol	350.07		NIST Webbook
tb	719.85	K	Joback Method
tc	990.35	K	Joback Method
tf	499.50	K	Joback 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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R173174&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

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