2-NITROFLUORANTHENE

Other names: 2-Nitrofluoranthene
Inchi: InChI=1S/C16H9NO2/c18-17(19)11-8-10-4-3-7-14-12-5-1-2-6-13(12)15(9-11)16(10)14/h
InchiKey: VBCBFNMZBHKVQN-UHFFFAOYSA-N
Formula: C16H9NO2
SMILES: O=[N+]([O-])c1cc2c3c(cccc3c1)-c1ccccc1-2
Mol. weight [g/mol]: 247.25

Physical Properties

Property code	Value	Unit	Source
hf	266.42	kJ/mol	Cheméo Relay (1.0)
hfus	35.47	kJ/mol	Joback Method
hvap	110.92	kJ/mol	Cheméo Relay (1.0)
ie	8.08	eV	Cheméo Relay (1.0)
log10ws	-5.88		Cheméo Relay (1.0)
logp	4.395		Crippen Method
mcvol	175.880	ml/mol	McGowan Method
rinpol	411.26		NIST Webbook
rinpol	411.85		NIST Webbook
rinpol	411.85		NIST Webbook
rinpol	412.48		NIST Webbook
rinpol	412.59		NIST Webbook
rinpol	411.26		NIST Webbook
rinpol	412.45		NIST Webbook
rinpol	412.45		NIST Webbook
tb	701.27	K	Cheméo Relay (1.0)
tf	439.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.39	J/mol×K	808.18	Joback Method
cpg	484.71	J/mol×K	853.89	Joback Method
cpg	495.53	J/mol×K	899.60	Joback Method
cpg	506.09	J/mol×K	945.31	Joback Method

cpg	516.66	J/mol×K	991.01	Joback Method
cpg	527.49	J/mol×K	1036.72	Joback Method
cpg	538.85	J/mol×K	1082.43	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13177292&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point