1-Nitrofluoranthene

Other names: Fluoranthene, 1-nitro-
7-Nitrofluoranthene
Inchi: InChI=1S/C16H9NO2/c18-17(19)14-9-8-10-4-3-7-12-11-5-1-2-6-13(11)16(14)15(10)12/h1
InchiKey: AWYZHUPAWKZJSL-UHFFFAOYSA-N
Formula: C16H9NO2
SMILES: O=[N+]([O-])c1ccc2cccc3c2c1-c1ccccc1-3
Mol. weight [g/mol]: 247.25
CAS: 13177-28-1

Physical Properties

Property code	Value	Unit	Source
gf	517.10	kJ/mol	Joback Method
hf	345.54	kJ/mol	Joback Method
hfus	35.47	kJ/mol	Joback Method
hvap	76.35	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	4.395		Crippen Method
mcvol	175.880	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	404.71		NIST Webbook
rinpol	404.37		NIST Webbook
tb	808.18	K	Joback Method
tc	1082.43	K	Joback Method
tf	582.05	K	Joback Method
vc	0.702	m3/kmol	Joback Method

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

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=C13177281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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