Fluoranthene, 3-nitro-

Other names:	3-Nitrofluoranthene
	4-Nitrofluoranthene
Inchi:	InChI=1S/C16H9NO2/c18-17(19)15-9-8-13-11-5-2-1-4-10(11)12-6-3-7-14(15)16(12)13/h
InchiKey:	PIHGQKMEAMSUNA-UHFFFAOYSA-N
Formula:	C16H9NO2
SMILES:	O=[N+]([O-])c1ccc2c3c(cccc13)-c1ccccc1-2
Mol. weight [g/mol]:	247.25
CAS:	892-21-7

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	411.89		NIST Webbook
rinpol	413.34		NIST Webbook
rinpol	419.80		NIST Webbook
rinpol	423.90		NIST Webbook
rinpol	413.33		NIST Webbook
rinpol	423.90		NIST Webbook
rinpol	412.45		NIST Webbook
rinpol	2433.00		NIST Webbook
rinpol	413.24		NIST Webbook
rinpol	411.89		NIST Webbook
rinpol	413.34		NIST Webbook
rinpol	412.45		NIST Webbook
rinpol	2433.00		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
hfust	22.60	kJ/mol	435.00	NIST Webbook

Sources

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=C892217&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
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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