1-Nitropyrene

Other names: 3-Nitropyrene
Pyrene, 1-nitro-
Inchi: InChI=1S/C16H9NO2/c18-17(19)14-9-7-12-5-4-10-2-1-3-11-6-8-13(14)16(12)15(10)11/h
InchiKey: ALRLPDGCPYIVHP-UHFFFAOYSA-N
Formula: C16H9NO2
SMILES: O=[N+]([O-])c1ccc2ccc3cccc4ccc1c2c34
Mol. weight [g/mol]: 247.25
CAS: 5522-43-0

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	-6.95		Crippen Method
logp	4.492		Crippen Method
mcvol	175.880	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	421.08		NIST Webbook
rinpol	425.50		NIST Webbook
rinpol	421.53		NIST Webbook
rinpol	420.60		NIST Webbook
rinpol	421.48		NIST Webbook
rinpol	419.25		NIST Webbook
rinpol	421.13		NIST Webbook
rinpol	421.18		NIST Webbook
rinpol	421.39		NIST Webbook
rinpol	421.48		NIST Webbook
rinpol	419.25		NIST Webbook
rinpol	421.08		NIST Webbook
rinpol	421.26		NIST Webbook
rinpol	421.27		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	516.66	J/mol×K	991.01	Joback Method
cpg	527.49	J/mol×K	1036.72	Joback Method
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	538.85	J/mol×K	1082.43	Joback Method
hfust	18.90	kJ/mol	425.90	NIST Webbook
hsubt	125.20 ± 3.80	kJ/mol	393.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5522430&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
hfust: Enthalpy of fusion at a given temperature
hsubt: Enthalpy of sublimation 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