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

Physical Properties

Property code	Value	Unit	Source
hf	236.24	kJ/mol	Cheméo Relay (1.0)
hfus	35.47	kJ/mol	Joback Method
hvap	107.17	kJ/mol	Cheméo Relay (1.0)
ie	7.74	eV	Cheméo Relay (1.0)
log10ws	-5.54		Cheméo Relay (1.0)
logp	4.492		Crippen Method
mcvol	175.880	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	421.39		NIST Webbook
rinpol	421.18		NIST Webbook
rinpol	421.26		NIST Webbook
rinpol	421.27		NIST Webbook
rinpol	425.50		NIST Webbook
rinpol	419.25		NIST Webbook
rinpol	419.25		NIST Webbook
rinpol	421.48		NIST Webbook
rinpol	421.53		NIST Webbook
rinpol	421.08		NIST Webbook
rinpol	421.13		NIST Webbook
rinpol	421.08		NIST Webbook
rinpol	420.60		NIST Webbook
rinpol	421.48		NIST Webbook
tb	712.87	K	Cheméo Relay (1.0)
tc	1072.97	K	Cheméo Relay (1.0)
tf	427.09	K	Cheméo Relay (1.0)
vc	0.659	m3/kmol	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
hfust	18.90	kJ/mol	425.90	NIST Webbook
hsubt	125.20 ± 3.80	kJ/mol	393.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

New method for determination of vaporization and sublimation enthalpy of aromatic compounds at 298.15 K using solution calorimetry technique and group-additivity scheme: https://www.doi.org/10.1016/j.tca.2015.09.022

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5522430&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
hfust: Enthalpy of fusion at a given temperature
hsubt: Enthalpy of sublimation at a given temperature
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume