

PYRENE, 4-NITRO-

Other names:	4-Nitropyrene
Inchi:	InChI=1S/C16H9NO2/c18-17(19)14-9-12-5-1-3-10-7-8-11-4-2-6-13(14)16(11)15(10)12/h
InchiKey:	UISKIUIWPSPSAV-UHFFFAOYSA-N
Formula:	C16H9NO2
SMILES:	O=[N+]([O-])c1cc2cccc3ccc4cccc1c4c32
Mol. weight [g/mol]:	247.25

Physical Properties

Property code	Value	Unit	Source
hf	243.63	kJ/mol	Cheméo Relay (1.0)
hfus	35.47	kJ/mol	Joback Method
hvap	105.01	kJ/mol	Cheméo Relay (1.0)
ie	7.74	eV	Cheméo Relay (1.0)
log10ws	-5.63		Cheméo Relay (1.0)
logp	4.492		Crippen Method
mcvol	175.880	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	415.64		NIST Webbook
rinpol	413.95		NIST Webbook
rinpol	415.52		NIST Webbook
rinpol	413.95		NIST Webbook
tb	710.76	K	Cheméo Relay (1.0)
tc	1074.62	K	Cheméo Relay (1.0)
tf	428.01	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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C57835924&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/97-854-7/PYRENE-4-NITRO.pdf>

Generated by Cheméo on 2026-07-21 18:10:11.901311502 +0000 UTC m=+168507.743196987.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.