

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
CAS:	57835-92-4

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	413.95		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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57835924&Units=SI

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

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