

6-NITROCHRYSENE

Other names:	Chrysene, 6-nitro-
Inchi:	InChI=1S/C18H11NO2/c20-19(21)18-11-17-13-6-2-1-5-12(13)9-10-15(17)14-7-3-4-8-16(2)H
InchiKey:	UAWLTQJFZUYROA-UHFFFAOYSA-N
Formula:	C18H11NO2
SMILES:	O=[N+]([O-])c1cc2c3ccccc3ccc2c2ccccc12
Mol. weight [g/mol]:	273.29

Physical Properties

Property code	Value	Unit	Source
hf	260.27	kJ/mol	Cheméo Relay (1.0)
hfus	37.67	kJ/mol	Joback Method
hvap	120.08	kJ/mol	Cheméo Relay (1.0)
ie	7.97	eV	Cheméo Relay (1.0)
log10ws	-6.46		Cheméo Relay (1.0)
logp	5.054		Crippen Method
mcvol	199.760	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	460.49		NIST Webbook
rinpol	463.60		NIST Webbook
rinpol	464.50		NIST Webbook
rinpol	463.60		NIST Webbook
rinpol	460.49		NIST Webbook
tb	748.03	K	Cheméo Relay (1.0)
tc	1101.40	K	Cheméo Relay (1.0)
tf	461.01	K	Cheméo Relay (1.0)
vc	0.727	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.44	J/mol×K	861.64	Joback Method
cpg	570.99	J/mol×K	908.23	Joback Method
cpg	582.94	J/mol×K	954.81	Joback Method
cpg	594.55	J/mol×K	1001.40	Joback Method

cpg	606.06	J/mol×K	1047.99	Joback Method
cpg	617.73	J/mol×K	1094.58	Joback Method
cpg	629.81	J/mol×K	1141.16	Joback Method
hfust	28.40	kJ/mol	486.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C7496028&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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

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