1-Naphthalenecarbonitrile

Other names:	1-Naphthalenenitrile
	1-Naphthylnitrile
	1-cyanonaphthalene
	1-naphthonitrile
	1-naphthyl cyanide
	NSC 60230
	Naphthalene-1-carbonitrile
	«alpha»-Cyanonaphthalene
	«alpha»-Naphthonitrile
	«alpha»-Naphthylnitrile
Inchi:	InChI=1S/C11H7N/c12-8-10-6-3-5-9-4-1-2-7-11(9)10/h1-7H
InchiKey:	YJMNOKOLADGBKA-UHFFFAOYSA-N
Formula:	C11H7N
SMILES:	N#Cc1cccc2ccccc12
Mol. weight [g/mol]:	153.18
CAS:	86-53-3

Physical Properties

Property code	Value	Unit	Source
chs	-5578.10	kJ/mol	NIST Webbook
ea	0.68 ± 0.10	eV	NIST Webbook
gf	384.35	kJ/mol	Joback Method
hf	310.64	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
ie	8.59	eV	NIST Webbook
ie	8.61	eV	NIST Webbook
log10ws	-3.63		Crippen Method
logp	2.711		Crippen Method
mcvol	124.010	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	256.75		NIST Webbook
rinpol	256.29		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1489.00		NIST Webbook

rinpol	1489.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	256.29		NIST Webbook
tb	572.20	K	NIST Webbook
tb	572.15 ± 2.00	K	NIST Webbook
tc	855.02	K	Joback Method
tf	308.65 ± 1.50	K	NIST Webbook
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.92	J/mol×K	603.80	Joback Method
cpg	286.01	J/mol×K	645.67	Joback Method
cpg	296.16	J/mol×K	687.54	Joback Method
cpg	305.46	J/mol×K	729.41	Joback Method
cpg	314.00	J/mol×K	771.28	Joback Method
cpg	321.87	J/mol×K	813.15	Joback Method
cpg	329.14	J/mol×K	855.02	Joback Method
hvapt	88.60	kJ/mol	298.13	Standard molar enthalpies of formation of 1- and 2-cyanonaphthalene

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Standard molar enthalpies of formation of 1- and 2-cyanonaphthalene: https://www.doi.org/10.1016/j.jct.2011.03.013

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=C86533&Units=SI

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
hvapt:	Enthalpy of vaporization at a given temperature
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