2-Naphthalenecarbonitrile

Other names:	2-Cyanonaphthalene
	2-Cyanonaphthylene
	2-Naphthalenenitrile
	2-naphthonitrile
	2-naphthyl cyanide
	Naphthalene-2-carbonitrile
	naphthalene, 2-cyano-
	«beta»-Cyanonaphthalene
	«beta»-Naphthonitrile
Inchi:	InChI=1S/C11H7N/c12-8-9-5-6-10-3-1-2-4-11(10)7-9/h1-7H
InchiKey:	AZKDTTQQTKDXLH-UHFFFAOYSA-N
Formula:	C11H7N
SMILES:	N#Cc1ccc2ccccc2c1
Mol. weight [g/mol]:	153.18
CAS:	613-46-7

Physical Properties

Property code	Value	Unit	Source
chs	-5553.40	kJ/mol	NIST Webbook
ea	0.65 ± 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	8.64	eV	NIST Webbook
ie	8.56	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	261.30		NIST Webbook
rinpol	261.50		NIST Webbook
rinpol	260.88		NIST Webbook
rinpol	1529.00		NIST Webbook
tb	579.65 ± 2.00	K	NIST Webbook
tb	579.70	K	NIST Webbook
tc	855.02	K	Joback Method

tf	332.15 ± 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	91.80	kJ/mol	306.14	Standard molar enthalpies of formation of 1- and 2-cyanonaphthalene

Sources

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=C613467&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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