1-Naphthalenecarboxaldehyde

Other names:	1-Naphthaldehyde
	«alpha»-Naphthaldehyde
	«alpha»-Naphthylaldehyde
	«alpha»-Naphthylcarboxaldehyde
	1-Formylnaphthalene
	1-Naphthylaldehyde
	«alpha»-Naphthal
	Naphthalene-1-carbaldehyde
	NSC 6106
	Naphthalene-1-carboxaldehyde
Inchi:	InChI=1S/C11H8O/c12-8-10-6-3-5-9-4-1-2-7-11(9)10/h1-8H
InchiKey:	SQAINHDHICKHLX-UHFFFAOYSA-N
Formula:	C11H8O
SMILES:	O=Cc1cccc2ccccc12
Mol. weight [g/mol]:	156.18
CAS:	66-77-3

Physical Properties

Property code	Value	Unit	Source
ea	0.74 ± 0.07	eV	NIST Webbook
ea	0.68 ± 0.02	eV	NIST Webbook
ea	0.68 ± 0.10	eV	NIST Webbook
gf	151.65	kJ/mol	Joback Method
hf	60.18	kJ/mol	Joback Method
hfus	17.21	kJ/mol	Joback Method
hvap	51.38	kJ/mol	Joback Method
ie	8.43 ± 0.03	eV	NIST Webbook
ie	8.33	eV	NIST Webbook
log10ws	-3.52		Crippen Method
logp	2.652		Crippen Method
mcvol	124.200	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	257.40		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	249.26		NIST Webbook
ripol	2364.00		NIST Webbook
tb	565.20	K	NIST Webbook

tc	788.21	K	Joback Method
tf	327.37	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.97	J/mol×K	550.38	Joback Method
cpg	281.39	J/mol×K	590.02	Joback Method
cpg	292.82	J/mol×K	629.66	Joback Method
cpg	303.33	J/mol×K	669.30	Joback Method
cpg	312.99	J/mol×K	708.93	Joback Method
cpg	321.89	J/mol×K	748.57	Joback Method
cpg	330.10	J/mol×K	788.21	Joback Method
dvisc	0.0018275	Pa×s	327.37	Joback Method
dvisc	0.0012484	Pa×s	364.54	Joback Method
dvisc	0.0009152	Pa×s	401.71	Joback Method
dvisc	0.0007071	Pa×s	438.88	Joback Method
dvisc	0.0005688	Pa×s	476.04	Joback Method
dvisc	0.0004722	Pa×s	513.21	Joback Method
dvisc	0.0004020	Pa×s	550.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	2.00	NIST Webbook

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=C66773&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume