2-Naphthalenecarboxaldehyde

Other names:	.beta.-naphthaldehyde
	2-Formylnaphthalene
	2-naphthaldehyde
	«beta»-Formylnaphthalene
	«beta»-Naphthaldehyde
	«beta»-Naphthylaldehyde
	«beta»-Naphthylcarboxaldehyde
Inchi:	InChI=1S/C11H8O/c12-8-9-5-6-10-3-1-2-4-11(10)7-9/h1-8H
InchiKey:	PJKVFARRVXDXAD-UHFFFAOYSA-N
Formula:	C11H8O
SMILES:	O=Cc1ccc2ccccc2c1
Mol. weight [g/mol]:	156.18
CAS:	66-99-9

Physical Properties

Property code	Value	Unit	Source
ea	0.62 ± 0.02	eV	NIST Webbook
ea	0.62 ± 0.04	eV	NIST Webbook
ea	0.64 ± 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
log10ws	-3.52		Crippen Method
logp	2.652		Crippen Method
mcvol	124.200	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	257.90		NIST Webbook
rinpol	259.10		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	258.20		NIST Webbook
rinpol	258.20		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	259.10		NIST Webbook
ripol	2407.00		NIST Webbook
ripol	2407.00		NIST Webbook
tb	550.38	K	Joback Method

tc	788.21	K	Joback Method
tf	333.27	K	Solubility Measurement and Correlation for 2-Naphthaldehyde in Pure Organic Solvents and Methanol + Ethanol Mixtures
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	2.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66999&Units=SI

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

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

Solid-liquid equilibrium and phase diagram for the ternary (2-naphthaldehyde + o-phthalic anhydride + 1,2-dichloroethane) system	https://www.doi.org/10.1016/j.jct.2016.06.011
Solubility Measurement and Correlation for 2-Naphthaldehyde in Pure Organic Solvents and Methanol + Ethanol Mixtures	https://www.doi.org/10.1021/acs.jced.5b00377
Solid-Liquid Phase Equilibria of the Ternary System (2-Naphthaldehyde + 4-Methylphthalic Anhydride + Ethyl Acetate) at (288.15, 298.15, and 308.15) K.	https://www.doi.org/10.1021/acs.jced.8b00170
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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