2-Naphthalenecarboxylic acid

Other names:	2-Naphthoic acid
	«beta»-Naphthoic acid
	Isonaphthoic acid
	2-Carboxynaphthalene
	2-Maythic acid
	2-Naphthioic acid
	Naphthalene-«beta»-carboxylic acid
	NSC 59901
	2-Naphthylcarboxylic acid
Inchi:	InChI=1S/C11H8O2/c12-11(13)10-6-5-8-3-1-2-4-9(8)7-10/h1-7H,(H,12,13)
InchiKey:	UOBYKYZJUGYBDK-UHFFFAOYSA-N
Formula:	C11H8O2
SMILES:	O=C(O)c1ccc2ccccc2c1
Mol. weight [g/mol]:	172.18
CAS:	93-09-4

Physical Properties

Property code	Value	Unit	Source
chs	-5125.90 ± 1.40	kJ/mol	NIST Webbook
chs	-5125.90 ± 1.40	kJ/mol	NIST Webbook
chs	-5138.00 ± 7.20	kJ/mol	NIST Webbook
gf	-14.57	kJ/mol	Joback Method
hf	-232.50 ± 1.70	kJ/mol	NIST Webbook
hfs	-346.10 ± 1.50	kJ/mol	NIST Webbook
hfus	20.60	kJ/mol	Joback Method
hsub	113.60	kJ/mol	NIST Webbook
hsub	117.19	kJ/mol	NIST Webbook
hsub	117.20	kJ/mol	NIST Webbook
hvap	68.08	kJ/mol	Joback Method
ie	8.26	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
log10ws	-3.34		Crippen Method
logp	2.538		Crippen Method
mcvol	130.070	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
rinpol	289.55		NIST Webbook
rinpol	289.55		NIST Webbook

tb	647.77	K	Joback Method
tc	870.83	K	Joback Method
tf	458.00 ± 3.00	K	NIST Webbook
tf	458.15 ± 2.00	K	NIST Webbook
tf	457.20 ± 1.50	K	NIST Webbook
tf	457.56 ± 0.35	K	NIST Webbook
tf	458.75 ± 0.25	K	NIST Webbook
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.65	J/mol×K	796.48	Joback Method
cpg	361.68	J/mol×K	870.83	Joback Method
cpg	354.92	J/mol×K	833.65	Joback Method
cpg	312.31	J/mol×K	647.77	Joback Method
cpg	322.21	J/mol×K	684.95	Joback Method
cpg	331.36	J/mol×K	722.12	Joback Method
cpg	339.82	J/mol×K	759.30	Joback Method
dvisc	0.0002426	Pa×s	563.89	Joback Method
dvisc	0.0001219	Pa×s	647.77	Joback Method
dvisc	0.0001679	Pa×s	605.83	Joback Method
dvisc	0.0023028	Pa×s	396.12	Joback Method
dvisc	0.0011161	Pa×s	438.06	Joback Method
dvisc	0.0006139	Pa×s	480.00	Joback Method
dvisc	0.0003718	Pa×s	521.94	Joback Method
hfust	23.54	kJ/mol	460.20	NIST Webbook
hfust	23.54	kJ/mol	460.20	NIST Webbook
hsubt	113.60 ± 0.80	kJ/mol	355.00	NIST Webbook
hsubt	113.60 ± 0.79	kJ/mol	355.60	NIST Webbook
hvapt	98.90	kJ/mol	522.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93094&Units=SI

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

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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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