1-Naphthalenecarboxylic acid

Other names:	1-Carboxynaphthalene
	1-Naphthioic acid
	1-Naphthoic acid
	Naphthalene-«alpha»-carboxylic acid
	Naphthalene-Â«alphaÂ»-carboxylic acid
	naphthoic acid
	«alpha»-Naphthoic acid
	«alpha»-Naphthylcarboxylic acid
	Â«alphaÂ»-Naphthoic acid
	Â«alphaÂ»-Naphthylcarboxylic acid
Inchi:	InChI=1S/C11H8O2/c12-11(13)10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,(H,12,13)
InchiKey:	LNETULKMXZVUST-UHFFFAOYSA-N
Formula:	C11H8O2
SMILES:	O=C(O)c1cccc2ccccc12
Mol. weight [g/mol]:	172.18
CAS:	86-55-5

Physical Properties

Property code	Value	Unit	Source
chs	-5110.70 ± 5.10	kJ/mol	NIST Webbook
chs	-5150.90 ± 6.70	kJ/mol	NIST Webbook
chs	-5138.41 ± 0.88	kJ/mol	NIST Webbook
chs	-5138.43 ± 0.87	kJ/mol	NIST Webbook
gf	-14.57	kJ/mol	Joback Method
hf	-223.10	kJ/mol	NIST Webbook
hfs	-333.50 ± 1.00	kJ/mol	NIST Webbook
hfus	20.60	kJ/mol	Joback Method
hsub	113.64	kJ/mol	NIST Webbook
hsub	110.40	kJ/mol	NIST Webbook
hsub	113.60	kJ/mol	NIST Webbook
hvap	68.08	kJ/mol	Joback Method
ie	8.29	eV	NIST Webbook
ie	8.29	eV	NIST Webbook
log10ws	-3.77		Aqueous Solubility Prediction Method
logp	2.538		Crippen Method
mcvol	130.070	ml/mol	McGowan Method

pc	4119.70	kPa	Joback Method
tb	573.20	K	NIST Webbook
tc	870.83	K	Joback Method
tf	433.90 ± 0.80	K	NIST Webbook
tf	434.48	K	Aqueous Solubility Prediction Method
tf	434.15 ± 2.00	K	NIST Webbook
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	347.65	J/mol×K	796.48	Joback Method
cpg	354.92	J/mol×K	833.65	Joback Method
cpg	361.68	J/mol×K	870.83	Joback Method
dvisc	0.0001219	Pa×s	647.77	Joback Method
dvisc	0.0011161	Pa×s	438.06	Joback Method
dvisc	0.0023028	Pa×s	396.12	Joback Method
dvisc	0.0003718	Pa×s	521.94	Joback Method
dvisc	0.0002426	Pa×s	563.89	Joback Method
dvisc	0.0001679	Pa×s	605.83	Joback Method
dvisc	0.0006139	Pa×s	480.00	Joback Method
hfust	19.89	kJ/mol	435.20	NIST Webbook
hfust	19.89	kJ/mol	435.20	NIST Webbook
hsubt	110.40 ± 0.20	kJ/mol	350.50	NIST Webbook
hsubt	110.40 ± 0.20	kJ/mol	350.00	NIST Webbook
hvapt	97.20	kJ/mol	515.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86555&Units=SI

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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