1-Naphthaleneacetic acid

Other names:

1-Naphthtaleneacetic acid
1-Naphthylacetic acid
1-naphthaceneacetic acid
1-naphthaleneethanoic acid
2-(1-Naphthyl)acetic acid
ANU
Agronaa
Alman
Alphaspra
Appl-Set
Biokor
Celmone
Etifix
Fruitofix
Fruitone N
Klingtite
Liqui-Stik
N 10
NAA
NSC 15772
Nafusaku
Naphthalene-1-acetic acid
Naphthaleneacetic acid
Naphthylacetic acid
Naphyl-1-essigsaeure
Niagara-Stik
Nu-Tone
Phymone
Phyomone
Pimacol-Sol
Planofix
Planofixe
Pomoxon
Primacol
Rasin
Rhizopon B
Rhodofix
Stafast
Stop-Drop
Tekkam

	Tip-Off
	Transplantone
	Tre-hold
	Vardhak
	ethanoic acid, 1-naphthalene-
	«alpha»-NAA
	«alpha»-Naphthaleneacetic acid
	«alpha»-Naphthylacetic acid
	«alpha»-Naphthyleneacetic acid
	Â«alphaÂ»-NAA
	Â«alphaÂ»-Naphthaleneacetic acid
	Â«alphaÂ»-Naphthylacetic acid
	Â«alphaÂ»-Naphthyleneacetic acid
Inchi:	InChI=1S/C12H10O2/c13-12(14)8-10-6-3-5-9-4-1-2-7-11(9)10/h1-7H,8H2,(H,13,14)
InchiKey:	PRPINYUDVPFIRX-UHFFFAOYSA-N
Formula:	C12H10O2
SMILES:	O=C(O)Cc1cccc2ccccc12
Mol. weight [g/mol]:	186.21
CAS:	86-87-3

Physical Properties

Property code	Value	Unit	Source
chs	-5792.09 ± 0.79	kJ/mol	NIST Webbook
gf	-6.15	kJ/mol	Joback Method
hf	-139.69	kJ/mol	Joback Method
hfs	-359.19 ± 0.79	kJ/mol	NIST Webbook
hfus	23.19	kJ/mol	Joback Method
hsub	112.30 ± 0.90	kJ/mol	NIST Webbook
hvap	70.31	kJ/mol	Joback Method
ie	7.71	eV	NIST Webbook
ie	7.99	eV	NIST Webbook
log10ws	-2.65		Aqueous Solubility Prediction Method
logp	2.467		Crippen Method
mcvol	144.160	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	670.65	K	Joback Method
tc	889.80	K	Joback Method
tf	406.48	K	Aqueous Solubility Prediction Method

tf	403.06	K	Solubility Measurement and the Correlation of 1-Naphthaleneacetic Acid in Pure and Methanol + Water Binary Solvents from T = (278.25 to 323.55) K
tf	405.95 ± 0.20	K	NIST Webbook
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.42	J/mol×K	670.65	Joback Method
cpg	371.04	J/mol×K	707.18	Joback Method
cpg	380.90	J/mol×K	743.70	Joback Method
cpg	390.05	J/mol×K	780.23	Joback Method
cpg	398.56	J/mol×K	816.75	Joback Method
cpg	406.48	J/mol×K	853.28	Joback Method
cpg	413.90	J/mol×K	889.80	Joback Method
dvisc	0.0009977	Pa×s	451.27	Joback Method
dvisc	0.0020861	Pa×s	407.39	Joback Method
dvisc	0.0005438	Pa×s	495.14	Joback Method
dvisc	0.0003271	Pa×s	539.02	Joback Method
dvisc	0.0002125	Pa×s	582.90	Joback Method
dvisc	0.0001466	Pa×s	626.77	Joback Method
dvisc	0.0001062	Pa×s	670.65	Joback Method
hfust	22.26	kJ/mol	405.30	NIST Webbook
hfust	22.26	kJ/mol	405.30	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility Measurement and the Correlation of 1-Naphthaleneacetic Acid in Pure and Methanol + Water Binary Solvents from T = (278.25 to 323.55) K:	https://www.doi.org/10.1021/acs.jced.6b00816

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