2-Naphthaleneacetic acid

Other names:	«beta»-Naphthaleneacetic acid
	2-(2-Naphthyl)acetic acid
	2-Naphthylacetic acid
	«beta»-Naphthylacetic acid
	Betoxan
	Acide «beta»-naphthylacetique
Inchi:	InChI=1S/C12H10O2/c13-12(14)8-9-5-6-10-3-1-2-4-11(10)7-9/h1-7H,8H2,(H,13,14)
InchiKey:	VIBOGIYPPWLDTI-UHFFFAOYSA-N
Formula:	C12H10O2
SMILES:	O=C(O)Cc1ccc2ccccc2c1
Mol. weight [g/mol]:	186.21
CAS:	581-96-4

Physical Properties

Property code	Value	Unit	Source
chs	-5779.34 ± 0.99	kJ/mol	NIST Webbook
gf	-6.15	kJ/mol	Joback Method
hf	-139.69	kJ/mol	Joback Method
hfs	-371.95 ± 0.99	kJ/mol	NIST Webbook
hfus	23.19	kJ/mol	Joback Method
hsub	124.60 ± 1.00	kJ/mol	NIST Webbook
hvap	70.31	kJ/mol	Joback Method
ie	8.05	eV	NIST Webbook
log10ws	-3.18		Crippen 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	407.39	K	Joback Method
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	0.0020861	Pa×s	407.39	Joback Method
dvisc	0.0009977	Pa×s	451.27	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

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=C581964&Units=SI

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
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