1,1'-BIPHENYL, 2-CARBOXY ACID

Other names:	o-Phenylbenzoic acid
	Biphenyl-2-carboxylic acid
	Biphenylcarboxylic acid-(2)
	[1,1'-Biphenyl]-2-carboxylic acid
	Diphenyl-2-carboxylic acid
	2-Phenylbenzoic acid
Inchi:	InChI=1S/C13H10O2/c14-13(15)12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H,(H,14,15)
InchiKey:	ILYSAKHOYBPSPC-UHFFFAOYSA-N
Formula:	C13H10O2
SMILES:	O=C(O)c1ccccc1-c1ccccc1
Mol. weight [g/mol]:	198.22

Physical Properties

Property code	Value	Unit	Source
af	0.7137		Cheméo Relay (1.0)
chs	-6195.70 ± 6.30	kJ/mol	NIST Webbook
gf	8.03	kJ/mol	Joback Method
hf	-188.90	kJ/mol	Cheméo Relay (1.0)
hfus	22.81	kJ/mol	Joback Method
hsub	121.30 ± 4.30	kJ/mol	NIST Webbook
hvap	102.21	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-3.19		Cheméo Relay (1.0)
logp	3.052		Crippen Method
mcvol	153.950	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	616.70	K	NIST Webbook
tb	616.50 ± 0.50	K	NIST Webbook
tc	901.63	K	Cheméo Relay (1.0)
tf	384.00 ± 3.00	K	NIST Webbook
tf	382.00 ± 3.00	K	NIST Webbook
tf	387.00	K	NIST Webbook
vc	0.550	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.95	J/mol×K	701.23	Joback Method
cpg	401.41	J/mol×K	739.68	Joback Method
cpg	411.94	J/mol×K	778.13	Joback Method
cpg	421.61	J/mol×K	816.58	Joback Method
cpg	430.47	J/mol×K	855.04	Joback Method
cpg	438.58	J/mol×K	893.49	Joback Method
cpg	445.99	J/mol×K	931.94	Joback Method
dvisc	0.0017023	Pa×s	412.38	Joback Method
dvisc	0.0006982	Pa×s	460.52	Joback Method
dvisc	0.0003390	Pa×s	508.66	Joback Method
dvisc	0.0001865	Pa×s	556.81	Joback Method
dvisc	0.0001128	Pa×s	604.95	Joback Method
dvisc	0.0000735	Pa×s	653.09	Joback Method
dvisc	0.0000508	Pa×s	701.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	472.20	K	1.30	NIST Webbook

Sources

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C947842&Units=SI

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

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

Legend

af:	Acentric Factor
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume