BIPHENYL-4-CARBOXYLIC ACID

Other names: 4-Biphenylcarboxylic acid
4-Carboxy-1,1'-biphenyl
4-Carboxybiphenyl
4-Diphenylcarboxylic acid
4-Phenylbenzoic acid
Benzoic acid, p-phenyl-
Biphenylcarboxylic acid-(4)
Diphenyl-4-carboxylic acid
NSC 23040
Para phenyl benzoic acid
[1,1'-Biphenyl]-4-carboxylic acid
p-Phenylbenzoic acid

Inchi: InChI=1S/C13H10O2/c14-13(15)12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H,(H,14,15)

InchiKey: NNJMFJSKMRYHSR-UHFFFAOYSA-N

Formula: C13H10O2

SMILES: O=C(O)c1ccc(-c2ccccc2)cc1

Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
af	0.7241		Cheméo Relay (1.0)
gf	8.03	kJ/mol	Joback Method
hf	-201.37	kJ/mol	Cheméo Relay (1.0)
hfus	22.81	kJ/mol	Joback Method
hsub	127.50 ± 4.10	kJ/mol	NIST Webbook
hvap	114.83	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-3.61		Cheméo Relay (1.0)
logp	3.052		Crippen Method
mcvol	153.950	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	618.09	K	Cheméo Relay (1.0)
tc	900.55	K	Cheméo Relay (1.0)
tf	483.00 ± 5.00	K	NIST Webbook
vc	0.555	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	445.99	J/mol×K	931.94	Joback Method
cpg	438.58	J/mol×K	893.49	Joback Method
cpg	430.47	J/mol×K	855.04	Joback Method
cpg	421.61	J/mol×K	816.58	Joback Method
cpg	411.94	J/mol×K	778.13	Joback Method
cpg	401.41	J/mol×K	739.68	Joback Method
dvisc	0.0001865	Pa×s	556.81	Joback Method
dvisc	0.0000508	Pa×s	701.23	Joback Method
dvisc	0.0000735	Pa×s	653.09	Joback Method
dvisc	0.0001128	Pa×s	604.95	Joback Method
dvisc	0.0017023	Pa×s	412.38	Joback Method
dvisc	0.0003390	Pa×s	508.66	Joback Method
dvisc	0.0006982	Pa×s	460.52	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92922&Units=SI

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

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

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):

Legend

af: Acentric Factor

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