2,2'-BIPHENYLDICARBOXYLIC ACID

Other names: 2,2'-Bibenzoic acid
2,2'-Dicarboxybiphenyl
2,2'-Diphenic acid
Biphenyl-2,2'-dicarboxylic acid
Diphenic acid
Diphenyl-2,2'-dicarboxylic acid
NSC 1966
o,o'-Bibenzoic acid
o,o'-Diphenic acid

Inchi: InChI=1S/C14H10O4/c15-13(16)11-7-3-1-5-9(11)10-6-2-4-8-12(10)14(17)18/h1-8H,(H,15

InchiKey: GWZCCUDJHOGOSO-UHFFFAOYSA-N

Formula: C14H10O4

SMILES: O=C(O)c1ccccc1-c1ccccc1C(=O)O

Mol. weight [g/mol]: 242.23

Physical Properties

Property code	Value	Unit	Source
af	0.9387		Cheméo Relay (1.0)
gf	-258.92	kJ/mol	Joback Method
hf	-532.67	kJ/mol	Cheméo Relay (1.0)
hfus	30.69	kJ/mol	Joback Method
hsub	151.90 ± 3.50	kJ/mol	NIST Webbook
hvap	135.74	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-2.28		Aqueous Solubility Prediction Method
logp	2.750		Crippen Method
mcvol	175.480	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	619.61	K	Cheméo Relay (1.0)
tc	970.27	K	Cheméo Relay (1.0)
tf	504.40	K	Aqueous Solubility Prediction Method
vc	0.620	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.67	J/mol×K	875.14	Joback Method
cpg	527.79	J/mol×K	1096.05	Joback Method
cpg	522.86	J/mol×K	1059.24	Joback Method
cpg	517.43	J/mol×K	1022.42	Joback Method
cpg	511.44	J/mol×K	985.60	Joback Method
cpg	504.85	J/mol×K	948.78	Joback Method
cpg	497.61	J/mol×K	911.96	Joback Method
dvisc	0.0000220	Pa×s	711.03	Joback Method
dvisc	0.0000051	Pa×s	875.14	Joback Method
dvisc	0.0000078	Pa×s	820.44	Joback Method
dvisc	0.0000126	Pa×s	765.73	Joback Method
dvisc	0.0002265	Pa×s	546.92	Joback Method
dvisc	0.0000420	Pa×s	656.33	Joback Method
dvisc	0.0000904	Pa×s	601.62	Joback Method
hsubt	166.10	kJ/mol	463.00	NIST Webbook

Sources

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C482053&Units=SI

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
hsubt:	Enthalpy of sublimation at a given temperature
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