

[1,1'-Biphenyl]-2,2'-dicarboxylic acid

Other names:

2,2'-Bibenzoic acid
2,2'-Biphenyldicarboxylic 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

CAS:

482-05-3

Physical Properties

Property code	Value	Unit	Source
gf	-258.92	kJ/mol	Joback Method
hf	-411.79	kJ/mol	Joback Method
hfus	30.69	kJ/mol	Joback Method
hsub	151.90 ± 3.50	kJ/mol	NIST Webbook
hvap	99.48	kJ/mol	Joback Method
log10ws	-2.28		Aqueous Solubility Prediction Method
logp	2.750		Crippen Method
mvol	175.480	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	875.14	K	Joback Method
tc	1096.05	K	Joback Method
tf	504.40	K	Aqueous Solubility Prediction Method
vc	0.653	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

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=C482053&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

Legend

- 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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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