Diphenylacetic acid

Other names:	.alpha.-phenylbenzeneacetic acid
	.alpha.-phenylbenzeneethanoic acid
	2,2-diphenylethanoic acid
	DPA
	acetic acid, diphenyl-
	benzeneacetic acid, .alpha.-phenyl-
	diphenylethanoic acid
	ethanoic acid, diphenyl-
	«alpha»,«alpha»-Diphenylacetic acid
	«alpha»-Toluic acid, «alpha»-phenyl-
Inchi:	InChI=1S/C14H12O2/c15-14(16)13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13H,(H,15,1
InchiKey:	PYHXGXCGESYPCW-UHFFFAOYSA-N
Formula:	C14H12O2
SMILES:	O=C(O)C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	212.25

Physical Properties

Property code	Value	Unit	Source
af	0.6667		Cheméo Relay (1.0)
gf	23.64	kJ/mol	Joback Method
hf	-214.88	kJ/mol	Cheméo Relay (1.0)
hfus	22.26	kJ/mol	Joback Method
hvap	46.74	kJ/mol	NIST Webbook
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-3.22		Aqueous Solubility Prediction Method
logp	2.903		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	591.32	K	Cheméo Relay (1.0)
tc	895.14	K	Cheméo Relay (1.0)
tf	419.90	K	Aqueous Solubility Prediction Method
tf	420.15 ± 1.00	K	NIST Webbook
tf	420.75 ± 0.20	K	NIST Webbook
tf	420.70 ± 1.50	K	NIST Webbook
tf	419.00 ± 3.00	K	NIST Webbook

tf	420.30	K	The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters
tt	420.44 ± 0.01	K	NIST Webbook
vc	0.578	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.76	J/mol×K	718.69	Joback Method
cpg	503.12	J/mol×K	948.69	Joback Method
cpg	495.13	J/mol×K	910.35	Joback Method
cpg	486.41	J/mol×K	872.02	Joback Method
cpg	476.88	J/mol×K	833.69	Joback Method
cpg	466.48	J/mol×K	795.36	Joback Method
cpg	455.12	J/mol×K	757.02	Joback Method
dvisc	0.0001003	Pa×s	611.17	Joback Method
dvisc	0.0000405	Pa×s	718.69	Joback Method
dvisc	0.0000615	Pa×s	664.93	Joback Method
dvisc	0.0026796	Pa×s	396.13	Joback Method
dvisc	0.0001797	Pa×s	557.41	Joback Method
dvisc	0.0003650	Pa×s	503.65	Joback Method
dvisc	0.0008779	Pa×s	449.89	Joback Method
hfust	31.25	kJ/mol	420.40	NIST Webbook
hfust	31.25	kJ/mol	420.40	NIST Webbook
hfust	31.18	kJ/mol	420.40	NIST Webbook

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters: https://www.doi.org/10.1016/j.tca.2012.03.028

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C117340&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
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
hfust:	Enthalpy of fusion 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
tt:	Triple Point Temperature
vc:	Critical Volume