

Benzeneacetic acid, «alpha»-phenyl-

Other names:	.alpha.-phenylbenzeneacetic acid .alpha.-phenylbenzeneethanoic acid 2,2-diphenylethanoic acid Acetic acid, diphenyl- DPA Diphenylacetic acid Diphenylethanoic acid benzeneacetic acid, .alpha.-phenyl- ethanoic acid, diphenyl- «alpha», «alpha»-Diphenylacetic acid «alpha»-Toluic acid, «alpha»-phenyl- Â«alphaÂ», Â«alphaÂ»-Diphenylacetic acid Â«alphaÂ»-Toluic acid, Â«alphaÂ»-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]:	212.24
CAS:	117-34-0

Physical Properties

Property code	Value	Unit	Source
gf	23.64	kJ/mol	Joback Method
hf	-129.32	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	46.74	kJ/mol	NIST Webbook
log10ws	-3.22		Aqueous Solubility Prediction Method
logp	2.903		Crippen Method
mccvol	168.040	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	718.69	K	Joback Method
tc	948.69	K	Joback Method
tf	420.75 ± 0.20	K	NIST Webbook

tf	420.30	K	The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters
tf	419.90	K	Aqueous Solubility Prediction Method
tf	420.70 ± 1.50	K	NIST Webbook
tf	420.15 ± 1.00	K	NIST Webbook
tf	419.00 ± 3.00	K	NIST Webbook
tt	420.44 ± 0.01	K	NIST Webbook
vc	0.623	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters:
Joback Method:

<https://www.doi.org/10.1016/j.tca.2012.03.028>

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

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C117340&Units=SI>

Crippen Method:

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

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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