Benzenebutanoic acid

Other names:	4-Phenyl-n-butyric acid
	4-Phenylbutanoic acid
	4-Phenylbutyric acid
	Benzenebutyric acid
	Butyric acid, 4-phenyl-
	Phenylbutyric acid
	butanoic acid, 4-phenyl-
	«gamma»-Phenyl-n-butyric acid
	«gamma»-Phenylbutyric acid
	«omega»-Phenylbutanoic acid
	Â«gammaÂ»-Phenyl-n-butyric acid
	Â«gammaÂ»-Phenylbutyric acid
	Â«omegaÂ»-Phenylbutanoic acid
Inchi:	InChI=1S/C10H12O2/c11-10(12)8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H,11,12)
InchiKey:	OBKXEAXTFZPCHS-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	O=C(O)CCCc1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	1821-12-1

Physical Properties

Property code	Value	Unit	Source
gf	-120.01	kJ/mol	Joback Method
hf	-278.01	kJ/mol	Joback Method
hfus	21.38	kJ/mol	Joback Method
hsub	113.00 ± 1.00	kJ/mol	NIST Webbook
hvap	63.55	kJ/mol	Joback Method
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-2.00		Aqueous Solubility Prediction Method
logp	2.094		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3210.00	kPa	Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids
rinpol	244.61		NIST Webbook
rinpol	244.61		NIST Webbook

rinpol	1417.00		NIST Webbook
tb	563.20	K	NIST Webbook
tc	801.20	K	Joback Method
tf	323.90	K	Aqueous Solubility Prediction Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.63	J/mol×K	767.82	Joback Method
cpg	385.80	J/mol×K	801.20	Joback Method
cpg	327.65	J/mol×K	600.93	Joback Method
cpg	338.96	J/mol×K	634.31	Joback Method
cpg	349.58	J/mol×K	667.69	Joback Method
cpg	359.54	J/mol×K	701.07	Joback Method
cpg	368.88	J/mol×K	734.44	Joback Method
dvisc	0.0000921	Pa×s	600.93	Joback Method
dvisc	0.0001406	Pa×s	557.38	Joback Method
dvisc	0.0059165	Pa×s	339.63	Joback Method
dvisc	0.0019932	Pa×s	383.18	Joback Method
dvisc	0.0008385	Pa×s	426.73	Joback Method
dvisc	0.0004141	Pa×s	470.28	Joback Method
dvisc	0.0002305	Pa×s	513.83	Joback Method
hfust	19.50	kJ/mol	324.20	NIST Webbook
hsubt	112.40 ± 0.80	kJ/mol	316.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.20	K	1.30	NIST Webbook

Sources

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1821121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids:	https://www.doi.org/10.1021/je060078g
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume