

Benzeneacetic acid

Other names:	2-Phenylacetic acid Acetic acid, phenyl- Benzenacetic acid Kyselina fenyloctova NSC 125718 Phenylacetic acid Phenylethanoic acid benzeneethanoic acid «alpha»-Toluic acid «omega»-Phenylacetic acid Â«alphaÂ»-Toluic acid Â«omegaÂ»-Phenylacetic acid
Inchi:	InChI=1S/C8H8O2/c9-8(10)6-7-4-2-1-3-5-7/h1-5H,6H2,(H,9,10)
InchiKey:	WLJVXDMOQOGPHL-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	O=C(O)Cc1ccccc1
Mol. weight [g/mol]:	136.15
CAS:	103-82-2

Physical Properties

Property code	Value	Unit	Source
chs	-3910.00	kJ/mol	NIST Webbook
chs	-3905.00	kJ/mol	NIST Webbook
chs	-3897.00	kJ/mol	NIST Webbook
chs	-3896.70 ± 0.80	kJ/mol	NIST Webbook
gf	-136.85	kJ/mol	Joback Method
hf	-236.73	kJ/mol	Joback Method
hfus	16.20	kJ/mol	Joback Method
hsub	93.50 ± 0.30	kJ/mol	NIST Webbook
hsub	99.00 ± 0.60	kJ/mol	NIST Webbook
hvap	79.10 ± 0.30	kJ/mol	NIST Webbook
ie	8.26	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
ie	8.26	eV	NIST Webbook

log10ws	-0.89	Aqueous Solubility Prediction Method	
logp	1.314	Crippen Method	
mcvol	107.260	ml/mol	McGowan Method
pc	3950.00	kPa	Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids
rinpol	1265.00	NIST Webbook	
rinpol	1263.00	NIST Webbook	
rinpol	1255.00	NIST Webbook	
rinpol	1248.00	NIST Webbook	
rinpol	1251.00	NIST Webbook	
rinpol	1248.00	NIST Webbook	
rinpol	1265.00	NIST Webbook	
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rinpol	1263.00	NIST Webbook	
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ripol	2565.00		NIST Webbook
ripol	2548.00		NIST Webbook
ripol	2548.00		NIST Webbook
ripol	2568.00		NIST Webbook
tb	538.70	K	NIST Webbook
tc	761.48	K	Joback Method
tf	348.05 ± 0.60	K	NIST Webbook
tf	350.00 ± 2.00	K	NIST Webbook
tf	349.15 ± 1.00	K	NIST Webbook
tf	348.00 ± 2.00	K	NIST Webbook
tf	350.32	K	Aqueous Solubility Prediction Method

vc	0.401	m3/kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.77	J/mol×K	555.17	Joback Method
cpg	246.37	J/mol×K	589.55	Joback Method
cpg	255.36	J/mol×K	623.94	Joback Method
cpg	263.77	J/mol×K	658.32	Joback Method
cpg	271.61	J/mol×K	692.71	Joback Method
cpg	278.92	J/mol×K	727.09	Joback Method
cpg	285.72	J/mol×K	761.48	Joback Method
dvisc	0.0001265	Pa×s	555.17	Joback Method
dvisc	0.0027201	Pa×s	356.77	Joback Method
dvisc	0.0011519	Pa×s	396.45	Joback Method
dvisc	0.0079644	Pa×s	317.09	Joback Method
dvisc	0.0003175	Pa×s	475.81	Joback Method
dvisc	0.0001935	Pa×s	515.49	Joback Method
dvisc	0.0005703	Pa×s	436.13	Joback Method
hfust	15.20	kJ/mol	349.20	NIST Webbook
hfust	16.50	kJ/mol	350.80	NIST Webbook
hfust	14.49	kJ/mol	349.90	NIST Webbook
hfust	14.49	kJ/mol	349.90	NIST Webbook
hsubt	98.60 ± 0.40	kJ/mol	313.00	NIST Webbook
hvapt	65.00	kJ/mol	454.50	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C103822&Units=SI>

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

Thermochemistry of phenylacetic and monochlorophenylacetic acids: <https://www.doi.org/10.1016/j.jct.2007.07.010>

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/AqueousDataset002.xlsx>

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

Legend

chs:	Standard solid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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