Benzeneacetic acid, «alpha»-methyl-

Other names:	2-Phenylpropionic acid
	2-Phenylpropanoic acid
	«alpha»-Phenylpropionic acid
	«alpha»-Methylphenylacetic acid
	Hydratropic acid
	dl-«alpha»-Phenylpropionic acid
	«alpha»-Methylbenzeneacetic acid
	Propanoic acid, 2-phenyl
Inchi:	InChI=1S/C9H10O2/c1-7(9(10)11)8-5-3-2-4-6-8/h2-7H,1H3,(H,10,11)
InchiKey:	YPGCWEMNNLXISK-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CC(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	150.17
CAS:	492-37-5

Physical Properties

Property code	Value	Unit	Source
gf	-130.87	kJ/mol	Joback Method
hf	-262.65	kJ/mol	Joback Method
hfus	15.27	kJ/mol	Joback Method
hvap	60.94	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.875		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
tb	534.20	K	NIST Webbook
tc	785.00	K	Joback Method
tf	313.36	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.79	J/mol×K	577.61	Joback Method
cpg	292.57	J/mol×K	612.17	Joback Method
cpg	302.67	J/mol×K	646.74	Joback Method
cpg	312.10	J/mol×K	681.30	Joback Method
cpg	320.91	J/mol×K	715.87	Joback Method
cpg	329.12	J/mol×K	750.43	Joback Method
cpg	336.75	J/mol×K	785.00	Joback Method
dvisc	0.0107638	Pa×s	313.36	Joback Method
dvisc	0.0030643	Pa×s	357.40	Joback Method
dvisc	0.0011492	Pa×s	401.44	Joback Method
dvisc	0.0005232	Pa×s	445.49	Joback Method
dvisc	0.0002745	Pa×s	489.53	Joback Method
dvisc	0.0001602	Pa×s	533.57	Joback Method
dvisc	0.0001014	Pa×s	577.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.50 ± 0.50	K	1.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C492375&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hvap:	Enthalpy of vaporization at standard conditions
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

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