Benzeneacetic acid, 4-methoxy-

Other names:	(4-Methoxyphenyl)acetic acid
	(4-methoxyphenyl)ethanoic acid
	(p-Methoxyphenyl)acetic acid
	2-(p-Anisyl)acetic acid
	4-Methoxybenzeneacetic acid
	4-methoxybenzeneethanoic acid
	4-methoxyphenylacetic acid
	Acetic acid, (p-methoxyphenyl)-
	Homoanisic acid
	MOPA
	NSC 27799
	ethanoic acid, (4-methoxyphenyl)-
	p-Anisylacetic acid
	p-Methoxy-«alpha»-toluic acid
	p-Methoxy-Â«alphaÂ»-toluic acid
Inchi:	InChI=1S/C9H10O3/c1-12-8-4-2-7(3-5-8)6-9(10)11/h2-5H,6H2,1H3,(H,10,11)
InchiKey:	NRPFNQUDKRYCNX-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1ccc(CC(=O)O)cc1
Mol. weight [g/mol]:	166.17
CAS:	104-01-8

Physical Properties

Property code	Value	Unit	Source
gf	-243.06	kJ/mol	Joback Method
hf	-401.06	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	64.40	kJ/mol	Joback Method
log10ws	-1.44		Aqueous Solubility Prediction Method
logp	1.322		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	1496.00		NIST Webbook
tb	605.45	K	Joback Method
tc	807.67	K	Joback Method

tf	358.05	K	Solubility Measurement, Modeling, and Thermodynamic Functions for para-Methoxyphenylacetic Acid in Pure and Mixed Organic and Aqueous Systems
tf	358.00 ± 0.50	K	NIST Webbook
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.17	J/mol×K	773.97	Joback Method
cpg	340.24	J/mol×K	740.27	Joback Method
cpg	331.76	J/mol×K	706.56	Joback Method
cpg	322.74	J/mol×K	672.86	Joback Method
cpg	313.16	J/mol×K	639.15	Joback Method
cpg	303.01	J/mol×K	605.45	Joback Method
cpg	355.59	J/mol×K	807.67	Joback Method
dvisc	0.0027550	Pa×s	363.11	Joback Method
dvisc	0.0000785	Pa×s	605.45	Joback Method
dvisc	0.0001149	Pa×s	565.06	Joback Method
dvisc	0.0001784	Pa×s	524.67	Joback Method
dvisc	0.0002980	Pa×s	484.28	Joback Method
dvisc	0.0005464	Pa×s	443.89	Joback Method
dvisc	0.0011315	Pa×s	403.50	Joback Method
hfust	21.80	kJ/mol	358.10	NIST Webbook
hfust	21.80	kJ/mol	358.10	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	0.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of cinnamic acid, phenoxyacetic acid and 4-methoxyphenylacetic acid in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2008.09.009
Solubility Measurement, Modeling, and Thermodynamic Functions for para-Methoxyphenylacetic Acid in Pure and Mixed Organic and Aqueous Systems:	https://www.doi.org/10.1021/acs.jced.8b00271
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
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
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