Benzeneacetic acid, 4-chloro-«alpha»-methyl-

Other names:	dl-p-Chloro-«alpha»-methylphenylacetic acid
	p-Chloro-«alpha»-methylphenylacetic acid
	4-Chloro-«alpha»-methylphenylacetic acid
	«alpha»-(p-Chlorophenyl)propionic acid
	p-Chloro-methylphenyl acetic acid
	2-(4-Chlorophenyl)propanoic acid
	DL-2-(4-chlorophenyl)propanoic acid
Inchi:	InChI=1S/C9H9ClO2/c1-6(9(11)12)7-2-4-8(10)5-3-7/h2-6H,1H3,(H,11,12)
InchiKey:	YOZILQVNIWNPFP-UHFFFAOYSA-N
Formula:	C9H9ClO2
SMILES:	CC(C(=O)O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	184.62
CAS:	938-95-4

Physical Properties

Property code	Value	Unit	Source
gf	-152.43	kJ/mol	Joback Method
hf	-289.86	kJ/mol	Joback Method
hfus	19.08	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.528		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1455.00		NIST Webbook
tb	620.02	K	Joback Method
tc	832.26	K	Joback Method
tf	355.80	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	303.58	J/mol×K	620.02	Joback Method
cpg	346.02	J/mol×K	796.89	Joback Method
cpg	338.71	J/mol×K	761.51	Joback Method
cpg	330.84	J/mol×K	726.14	Joback Method
cpg	322.38	J/mol×K	690.77	Joback Method
cpg	313.30	J/mol×K	655.39	Joback Method
cpg	352.80	J/mol×K	832.26	Joback Method
dvisc	0.0000849	Pa×s	620.02	Joback Method
dvisc	0.0001278	Pa×s	575.98	Joback Method
dvisc	0.0002057	Pa×s	531.95	Joback Method
dvisc	0.0003611	Pa×s	487.91	Joback Method
dvisc	0.0007084	Pa×s	443.87	Joback Method
dvisc	0.0016126	Pa×s	399.84	Joback Method
dvisc	0.0044996	Pa×s	355.80	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C938954&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

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
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume