Benzeneacetic acid, 4-chloro-

Other names:	(4-Chlorophenyl)acetic acid
	(4-chlorophenyl)ethanoic acid
	(p-Chlorophenyl)acetic acid
	2-(p-Chlorophenyl)acetic acid
	4-Chlorobenzeneacetic acid
	4-chlorobenzeneethanoic acid
	4-chlorophenylacetic acid
	Acetic acid, (p-chlorophenyl)-
	p-chlorophenylacetic acid
Inchi:	InChI=1S/C8H7ClO2/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4H,5H2,(H,10,11)
InchiKey:	CDPKJZJVTHSESZ-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	O=C(O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	170.59
CAS:	1878-66-6

Physical Properties

Property code	Value	Unit	Source
gf	-158.41	kJ/mol	Joback Method
hf	-263.94	kJ/mol	Joback Method
hfus	23.57	kJ/mol	Thermochemistry of phenylacetic and monochlorophenylacetic acids
hvap	64.15	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.967		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	597.58	K	Joback Method
tc	809.04	K	Joback Method
tf	359.53	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.49	J/mol×K	597.58	Joback Method
cpg	266.08	J/mol×K	632.82	Joback Method
cpg	274.10	J/mol×K	668.07	Joback Method
cpg	281.58	J/mol×K	703.31	Joback Method
cpg	288.55	J/mol×K	738.55	Joback Method
cpg	295.02	J/mol×K	773.80	Joback Method
cpg	301.02	J/mol×K	809.04	Joback Method
dvisc	0.0036481	Pa×s	359.53	Joback Method
dvisc	0.0015134	Pa×s	399.21	Joback Method
dvisc	0.0007361	Pa×s	438.88	Joback Method
dvisc	0.0004034	Pa×s	478.55	Joback Method
dvisc	0.0002425	Pa×s	518.23	Joback Method
dvisc	0.0001567	Pa×s	557.90	Joback Method
dvisc	0.0001073	Pa×s	597.58	Joback Method
hfust	23.57	kJ/mol	377.90	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1878666&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/18-410-6/Benzeneacetic-acid-4-chloro.pdf
Generated by Cheméo on 2024-04-17 19:07:03.894627221 +0000 UTC m=+15670072.815204533.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.