p-Chloromandelic acid

Other names:	4-Chloromandelic acid
	Benzeneacetic acid, 4-chloro-«alpha»-hydroxy-
	Mandelic acid, p-chloro-
	Para-chloromandelic acid
	4-Chloro-«alpha»-hydroxybenzeneethanoic acid
	NSC 31400
	DL-4-Chloromandelic acid
	(dl) p-chloromandelic acid
Inchi:	InChI=1S/C8H7ClO3/c9-6-3-1-5(2-4-6)7(10)8(11)12/h1-4,7,10H,(H,11,12)
InchiKey:	BWSFWXSSALIZAU-UHFFFAOYSA-N
Formula:	C8H7ClO3
SMILES:	O=C(O)C(O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	186.59
CAS:	492-86-4

Physical Properties

Property code	Value	Unit	Source
gf	-297.67	kJ/mol	Joback Method
hf	-421.45	kJ/mol	Joback Method
hfus	20.58	kJ/mol	Joback Method
hvap	80.44	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.458		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
pc	4743.15	kPa	Joback Method
tb	689.32	K	Joback Method
tc	891.12	K	Joback Method
tf	405.35	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.87	J/mol×K	689.32	Joback Method

cpg	303.93	J/mol×K	722.95	Joback Method
cpg	310.51	J/mol×K	756.59	Joback Method
cpg	316.62	J/mol×K	790.22	Joback Method
cpg	322.28	J/mol×K	823.85	Joback Method
cpg	327.53	J/mol×K	857.49	Joback Method
cpg	332.38	J/mol×K	891.12	Joback Method
dvisc	0.0028509	Pa×s	405.35	Joback Method
dvisc	0.0007972	Pa×s	452.68	Joback Method
dvisc	0.0002838	Pa×s	500.01	Joback Method
dvisc	0.0001207	Pa×s	547.34	Joback Method
dvisc	0.0000589	Pa×s	594.66	Joback Method
dvisc	0.0000319	Pa×s	641.99	Joback Method
dvisc	0.0000188	Pa×s	689.32	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C492864&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume