DL-P-CHLORO-ALPHA-HYDROXYPHENYLACETIC 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

Physical Properties

Property code	Value	Unit	Source
hf	-506.00	kJ/mol	Cheméo Relay (1.0)
hfus	20.58	kJ/mol	Joback Method
ie	9.01	eV	Cheméo Relay (1.0)
log10ws	-0.89		Cheméo Relay (1.0)
logp	1.458		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
tb	546.79	K	Cheméo Relay (1.0)
tf	412.58	K	Cheméo Relay (1.0)

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
hfust	27.20	kJ/mol	394.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C492864&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point