3-Chloro-2,6-dihydroxy-4-methylbenzaldehyde

Inchi: InChI=1S/C8H7ClO3/c1-4-2-6(11)5(3-10)8(12)7(4)9/h2-3,11-12H,1H3
InchiKey: IOTAGSGSURFFDS-UHFFFAOYSA-N
Formula: C8H7ClO3
SMILES: Cc1cc(O)c(C=O)c(O)c1Cl
Mol. weight [g/mol]: 186.59
CAS: 57074-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-311.06	kJ/mol	Joback Method
hf	-450.80	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	74.14	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.872		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1502.20		NIST Webbook
rinpol	1502.20		NIST Webbook
rinpol	1494.00		NIST Webbook
tb	666.41	K	Joback Method
tc	911.18	K	Joback Method
tf	526.74	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.31	J/mol×K	666.41	Joback Method
cpg	302.70	J/mol×K	707.21	Joback Method
cpg	309.66	J/mol×K	748.00	Joback Method
cpg	316.32	J/mol×K	788.80	Joback Method
cpg	322.83	J/mol×K	829.59	Joback Method

cpg	329.32	J/mol×K	870.39	Joback Method
cpg	335.92	J/mol×K	911.18	Joback Method
dvisc	0.0000518	Pa×s	526.74	Joback Method
dvisc	0.0000310	Pa×s	550.02	Joback Method
dvisc	0.0000193	Pa×s	573.30	Joback Method
dvisc	0.0000125	Pa×s	596.58	Joback Method
dvisc	0.0000084	Pa×s	619.85	Joback Method
dvisc	0.0000058	Pa×s	643.13	Joback Method
dvisc	0.0000041	Pa×s	666.41	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57074212&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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