2-CHLORO-9-HYDROXYFLUORENE-9-CARBOXYL ACID

Inchi: InChI=1S/C14H9ClO3/c15-8-5-6-10-9-3-1-2-4-11(9)14(18,13(16)17)12(10)7-8/h1-7,18H,(

InchiKey: SVOAUHHKPGKPQK-UHFFFAOYSA-N

Formula: C14H9ClO3

SMILES: O=C(O)C1(O)c2ccccc2-c2ccc(Cl)cc21

Mol. weight [g/mol]: 260.68

Physical Properties

Property code	Value	Unit	Source
gf	-72.10	kJ/mol	Joback Method
hf	-226.06	kJ/mol	Joback Method
hfus	28.94	kJ/mol	Joback Method
hvap	96.20	kJ/mol	Joback Method
log10ws	-4.18		Aqueous Solubility Prediction Method
logp	2.641		Crippen Method
mcvol	175.290	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
tb	862.12	K	Joback Method
tc	1086.49	K	Joback Method
tf	588.31	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.31	J/mol×K	862.12	Joback Method
cpg	484.31	J/mol×K	899.52	Joback Method
cpg	494.68	J/mol×K	936.91	Joback Method
cpg	505.62	J/mol×K	974.31	Joback Method
cpg	517.32	J/mol×K	1011.70	Joback Method
cpg	529.97	J/mol×K	1049.10	Joback Method
cpg	543.76	J/mol×K	1086.49	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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