4-Chloro-2,3,5,6-tetracarboxycyclohexadiene-2,5-

Inchi: InChI=1S/C10H5ClO9/c11-5-1(7(13)14)3(9(17)18)6(12)4(10(19)20)2(5)8(15)16/h5H,(H,1
InchiKey: LKHSBTWRNUYTOY-UHFFFAOYSA-N
Formula: C10H5ClO9
SMILES: O=C(O)C1=C(C(=O)O)C(Cl)C(C(=O)O)=C(C(=O)O)C1=O
Mol. weight [g/mol]: 304.59
CAS: 116277-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-1118.31	kJ/mol	Joback Method
hf	-1338.41	kJ/mol	Joback Method
hfus	40.83	kJ/mol	Joback Method
hvap	143.85	kJ/mol	Joback Method
log10ws	0.45		Crippen Method
logp	-0.892		Crippen Method
mcvol	175.870	ml/mol	McGowan Method
pc	5544.32	kPa	Joback Method
tb	1155.44	K	Joback Method
tc	1424.18	K	Joback Method
tf	802.58	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.79	J/mol×K	1155.44	Joback Method
cpg	489.40	J/mol×K	1200.23	Joback Method
cpg	486.41	J/mol×K	1245.02	Joback Method
cpg	481.78	J/mol×K	1289.81	Joback Method
cpg	475.46	J/mol×K	1334.60	Joback Method
cpg	467.41	J/mol×K	1379.39	Joback Method
cpg	457.60	J/mol×K	1424.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116277817&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
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