

1,2,3,5-Tetracarbomethoxy-5-chloro-4-methylcyclohexane

Inchi:	InChI=1S/C14H15ClO8/c1-6-7(10(16)20-2)8(11(17)21-3)9(12(18)22-4)14(6,15)13(19)23-
InchiKey:	KOFUVUOBYYWHSF-UHFFFAOYSA-N
Formula:	C14H15ClO8
SMILES:	<chem>COC(=O)C1=C(C)C(Cl)(C(=O)OC)C(C(=O)OC)=C1C(=O)OC</chem>
Mol. weight [g/mol]:	346.72
CAS:	93251-34-4

Physical Properties

Property code	Value	Unit	Source
gf	-828.15	kJ/mol	Joback Method
hf	-1181.83	kJ/mol	Joback Method
hfus	35.89	kJ/mol	Joback Method
hvap	90.11	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	0.283		Crippen Method
mcvol	230.660	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
tb	896.07	K	Joback Method
tc	1117.03	K	Joback Method
tf	652.50	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.54	J/molxK	896.07	Joback Method
cpg	674.74	J/molxK	932.90	Joback Method
cpg	686.48	J/molxK	969.72	Joback Method
cpg	697.79	J/molxK	1006.55	Joback Method
cpg	708.74	J/molxK	1043.38	Joback Method
cpg	719.37	J/molxK	1080.20	Joback Method
cpg	729.71	J/molxK	1117.03	Joback Method

Sources

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=C93251344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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