Dimethyl 2,3,4,4-tetrachloro-2-pentenedioate

Inchi: InChI=1S/C7H6Cl4O4/c1-14-5(12)3(8)4(9)7(10,11)6(13)15-2/h1-2H3/b4-3+
InchiKey: SBIOMHBKZIAVLQ-ONEGZZNKSA-N
Formula: C7H6Cl4O4
SMILES: COC(=O)C(Cl)=C(Cl)C(Cl)(Cl)C(=O)OC
Mol. weight [g/mol]: 295.93

Physical Properties

Property code	Value	Unit	Source
gf	-441.54	kJ/mol	Joback Method
hf	-651.48	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.196		Crippen Method
mcvol	169.030	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	662.55	K	Joback Method
tc	892.33	K	Joback Method
tf	402.07	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.71	J/mol×K	662.55	Joback Method
cpg	357.54	J/mol×K	700.85	Joback Method
cpg	364.71	J/mol×K	739.14	Joback Method
cpg	371.26	J/mol×K	777.44	Joback Method
cpg	377.23	J/mol×K	815.74	Joback Method
cpg	382.66	J/mol×K	854.03	Joback Method
cpg	387.57	J/mol×K	892.33	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=R80223&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume