Dimethyl 2-chloro-3-dichloromethylbutenedioate

Inchi: InChI=1S/C7H7Cl3O4/c1-13-6(11)3(5(9)10)4(8)7(12)14-2/h5H,1-2H3/b4-3-

InchiKey: JLBYWOCUVWNLJC-ARJAWSKDSA-N

Formula: C7H7Cl3O4

SMILES: COC(=O)C(Cl)=C(C(=O)OC)C(Cl)Cl

Mol. weight [g/mol]: 261.49

Physical Properties

Property code	Value	Unit	Source
gf	-434.89	kJ/mol	Joback Method
hf	-632.27	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	62.37	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.629		Crippen Method
mcvol	156.790	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	1425.00		NIST Webbook
tb	627.91	K	Joback Method
tc	846.17	K	Joback Method
tf	354.73	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.76	J/mol×K	627.91	Joback Method
cpg	335.36	J/mol×K	664.29	Joback Method
cpg	343.41	J/mol×K	700.66	Joback Method
cpg	350.93	J/mol×K	737.04	Joback Method
cpg	357.90	J/mol×K	773.42	Joback Method
cpg	364.35	J/mol×K	809.80	Joback Method
cpg	370.28	J/mol×K	846.17	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=R80269&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume