Succinic acid, 2-hydroxymethylene-3-isopropylidene-, diethyl ester

InChI: InChI=1S/C12H18O5/c1-5-16-11(14)9(7-13)10(8(3)4)12(15)17-6-2/h7,13H,5-6H2,1-4H3/
InChIKey: WCJJJAREEUKXEH-CLFYSBASSA-N
Formula: C12H18O5
SMILES: CCOC(=O)C(=CO)C(C(=O)OCC)=C(C)C
Mol. weight [g/mol]: 242.27
CAS: 95769-42-9

Physical Properties

Property code	Value	Unit	Source
gf	-419.71	kJ/mol	Joback Method
hf	-727.77	kJ/mol	Joback Method
hfus	32.97	kJ/mol	Joback Method
hvap	77.45	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.891		Crippen Method
mcvol	192.090	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	726.68	K	Joback Method
tc	917.20	K	Joback Method
tf	378.10	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.14	J/mol×K	726.68	Joback Method
cpg	539.90	J/mol×K	758.43	Joback Method
cpg	551.03	J/mol×K	790.19	Joback Method
cpg	561.54	J/mol×K	821.94	Joback Method
cpg	571.46	J/mol×K	853.69	Joback Method
cpg	580.81	J/mol×K	885.44	Joback Method
cpg	589.62	J/mol×K	917.20	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95769429&Units=SI

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