Succinic acid, dimethyl ester, 2-isopropylidene-3-(dimethoxymethylene)

Inchi: InChI=1S/C12H18O6/c1-7(2)8(10(13)15-3)9(11(14)16-4)12(17-5)18-6/h1-6H3
InchiKey: LKZWFRXXTRISRI-UHFFFAOYSA-N
Formula: C12H18O6
SMILES: COC(=O)C(=C(C)C)C(C(=O)OC)=C(OC)OC
Mol. weight [g/mol]: 258.27
CAS: 6414-72-8

Physical Properties

Property code	Value	Unit	Source
gf	-501.44	kJ/mol	Joback Method
hf	-849.77	kJ/mol	Joback Method
hfus	29.95	kJ/mol	Joback Method
hvap	65.67	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.173		Crippen Method
mcvol	197.960	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
tb	679.22	K	Joback Method
tc	878.02	K	Joback Method
tf	347.78	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.89	J/mol×K	679.22	Joback Method
cpg	538.73	J/mol×K	712.35	Joback Method
cpg	551.85	J/mol×K	745.49	Joback Method
cpg	564.24	J/mol×K	778.62	Joback Method
cpg	575.90	J/mol×K	811.75	Joback Method
cpg	586.82	J/mol×K	844.88	Joback Method
cpg	597.01	J/mol×K	878.02	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=C6414728&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