Dimethyl isopropylidene succinate

Inchi: InChI=1S/C9H14O4/c1-6(2)7(9(11)13-4)5-8(10)12-3/h5H2,1-4H3
InchiKey: MILMBEYRSAHUMS-UHFFFAOYSA-N
Formula: C9H14O4
SMILES: COC(=O)CC(C(=O)OC)=C(C)C
Mol. weight [g/mol]: 186.21
CAS: 87384-00-7

Physical Properties

Property code	Value	Unit	Source
gf	-379.82	kJ/mol	Joback Method
hf	-621.05	kJ/mol	Joback Method
hfus	22.22	kJ/mol	Joback Method
hvap	54.06	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.059		Crippen Method
mcvol	148.250	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
tb	561.82	K	Joback Method
tc	757.56	K	Joback Method
tf	302.51	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.40	J/mol×K	561.82	Joback Method
cpg	360.63	J/mol×K	594.44	Joback Method
cpg	372.29	J/mol×K	627.07	Joback Method
cpg	383.41	J/mol×K	659.69	Joback Method
cpg	393.99	J/mol×K	692.31	Joback Method
cpg	404.01	J/mol×K	724.93	Joback Method
cpg	413.51	J/mol×K	757.56	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=C87384007&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