Succinic acid, butyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C12H20O5/c1-4-5-8-16-11(14)6-7-12(15)17-10(3)9(2)13/h10H,4-8H2,1-3H3
InchiKey: COOOWMDTHVZDLQ-UHFFFAOYSA-N
Formula: C12H20O5
SMILES: CCCCOC(=O)CCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 244.28

Physical Properties

Property code	Value	Unit	Source
gf	-549.04	kJ/mol	Joback Method
hf	-898.47	kJ/mol	Joback Method
hfus	30.49	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.631		Crippen Method
mcvol	196.390	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1622.00		NIST Webbook
tb	679.97	K	Joback Method
tc	867.54	K	Joback Method
tf	404.25	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.62	J/mol×K	679.97	Joback Method
cpg	550.33	J/mol×K	711.23	Joback Method
cpg	563.33	J/mol×K	742.49	Joback Method
cpg	575.61	J/mol×K	773.75	Joback Method
cpg	587.17	J/mol×K	805.02	Joback Method
cpg	598.01	J/mol×K	836.28	Joback Method
cpg	608.13	J/mol×K	867.54	Joback Method
dvisc	0.0016566	Pa×s	404.25	Joback Method
dvisc	0.0008899	Pa×s	450.20	Joback Method

dvisc	0.0005364	Pa×s	496.16	Joback Method
dvisc	0.0003523	Pa×s	542.11	Joback Method
dvisc	0.0002471	Pa×s	588.06	Joback Method
dvisc	0.0001824	Pa×s	634.02	Joback Method
dvisc	0.0001403	Pa×s	679.97	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=U349579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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