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

Inchi: InChI=1S/C10H16O5/c1-4-14-9(12)5-6-10(13)15-8(3)7(2)11/h8H,4-6H2,1-3H3
InchiKey: IQLJYTQAAUIOTN-UHFFFAOYSA-N
Formula: C10H16O5
SMILES: CCOC(=O)CCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 216.23

Physical Properties

Property code	Value	Unit	Source
gf	-565.88	kJ/mol	Joback Method
hf	-857.19	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	0.850		Crippen Method
mcvol	168.210	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
tb	634.21	K	Joback Method
tc	825.12	K	Joback Method
tf	381.71	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.27	J/mol×K	634.21	Joback Method
cpg	446.78	J/mol×K	666.03	Joback Method
cpg	458.67	J/mol×K	697.85	Joback Method
cpg	469.95	J/mol×K	729.67	Joback Method
cpg	480.59	J/mol×K	761.48	Joback Method
cpg	490.60	J/mol×K	793.30	Joback Method
cpg	499.97	J/mol×K	825.12	Joback Method
dvisc	0.0019096	Pa×s	381.71	Joback Method

dvisc	0.0010572	Pa×s	423.79	Joback Method
dvisc	0.0006513	Pa×s	465.88	Joback Method
dvisc	0.0004348	Pa×s	507.96	Joback Method
dvisc	0.0003088	Pa×s	550.04	Joback Method
dvisc	0.0002302	Pa×s	592.13	Joback Method
dvisc	0.0001784	Pa×s	634.21	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=U349578&Units=SI

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