Succinic acid, 3-methylbut-2-yl but-3-en-1-yl ester

Inchi: InChI=1S/C13H22O4/c1-5-6-9-16-12(14)7-8-13(15)17-11(4)10(2)3/h5,10-11H,1,6-9H2,2-

InchiKey: QJUBXZHVTFKCOP-UHFFFAOYSA-N

Formula: C13H22O4

SMILES: C=CCCOC(=O)CCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-326.30	kJ/mol	Joback Method
hf	-686.38	kJ/mol	Joback Method
hfus	26.67	kJ/mol	Joback Method
hvap	61.40	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.474		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1532.00		NIST Webbook
rinpol	1532.00		NIST Webbook
tb	645.22	K	Joback Method
tc	829.76	K	Joback Method
tf	348.83	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.73	J/mol×K	645.22	Joback Method
cpg	561.85	J/mol×K	675.98	Joback Method
cpg	576.24	J/mol×K	706.73	Joback Method
cpg	589.89	J/mol×K	737.49	Joback Method
cpg	602.83	J/mol×K	768.24	Joback Method
cpg	615.04	J/mol×K	799.00	Joback Method
cpg	626.55	J/mol×K	829.76	Joback Method
dvisc	0.0024709	Pa×s	348.83	Joback Method

dvisc	0.0010978	Pa×s	398.23	Joback Method
dvisc	0.0005833	Pa×s	447.63	Joback Method
dvisc	0.0003515	Pa×s	497.03	Joback Method
dvisc	0.0002321	Pa×s	546.42	Joback Method
dvisc	0.0001642	Pa×s	595.82	Joback Method
dvisc	0.0001225	Pa×s	645.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391187&Units=SI
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

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