Succinic acid, 3-methylbut-2-yl pent-4-en-2-yl ester

Inchi: InChI=1S/C14H24O4/c1-6-7-11(4)17-13(15)8-9-14(16)18-12(5)10(2)3/h6,10-12H,1,7-9H2

InchiKey: MSDSGDINLMIMED-UHFFFAOYSA-N

Formula: C14H24O4

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

Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-320.32	kJ/mol	Joback Method
hf	-712.30	kJ/mol	Joback Method
hfus	25.74	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.862		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	1556.00		NIST Webbook
rinpol	1556.00		NIST Webbook
tb	667.66	K	Joback Method
tc	853.72	K	Joback Method
tf	345.10	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.34	J/mol×K	667.66	Joback Method
cpg	671.77	J/mol×K	822.71	Joback Method
cpg	659.07	J/mol×K	791.70	Joback Method
cpg	645.58	J/mol×K	760.69	Joback Method
cpg	631.30	J/mol×K	729.68	Joback Method
cpg	616.23	J/mol×K	698.67	Joback Method
cpg	683.70	J/mol×K	853.72	Joback Method
dvisc	0.0001005	Pa×s	667.66	Joback Method

dvisc	0.0001379	Pa×s	613.90	Joback Method
dvisc	0.0002011	Pa×s	560.14	Joback Method
dvisc	0.0003178	Pa×s	506.38	Joback Method
dvisc	0.0005597	Pa×s	452.62	Joback Method
dvisc	0.0011484	Pa×s	398.86	Joback Method
dvisc	0.0029477	Pa×s	345.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391153&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

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