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

Inchi: InChI=1S/C17H30O4/c1-6-8-9-10-15(7-2)21-17(19)12-11-16(18)20-14(5)13(3)4/h7,13-15

InchiKey: MUCONRDDMKUQDA-UHFFFAOYSA-N

Formula: C17H30O4

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

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-295.06	kJ/mol	Joback Method
hf	-774.22	kJ/mol	Joback Method
hfus	33.51	kJ/mol	Joback Method
hvap	69.91	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.032		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	736.30	K	Joback Method
tc	920.39	K	Joback Method
tf	378.91	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.31	J/mol×K	736.30	Joback Method
cpg	784.35	J/mol×K	766.98	Joback Method
cpg	800.46	J/mol×K	797.66	Joback Method
cpg	815.66	J/mol×K	828.35	Joback Method
cpg	829.96	J/mol×K	859.03	Joback Method
cpg	843.38	J/mol×K	889.71	Joback Method
cpg	855.92	J/mol×K	920.39	Joback Method
dvisc	0.0021329	Pa×s	378.91	Joback Method

dvisc	0.0008113	Pa×s	438.48	Joback Method
dvisc	0.0003889	Pa×s	498.04	Joback Method
dvisc	0.0002181	Pa×s	557.61	Joback Method
dvisc	0.0001368	Pa×s	617.17	Joback Method
dvisc	0.0000931	Pa×s	676.73	Joback Method
dvisc	0.0000675	Pa×s	736.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391317&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