

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

Inchi:	InChI=1S/C17H30O4/c1-6-7-8-9-10-14(4)20-16(18)11-12-17(19)21-15(5)13(2)3/h9-10,13
InchiKey:	VTNRJXUGNISTDW-MDZDMXLPSA-N
Formula:	C17H30O4
SMILES:	CCCCC=CC(C)OC(=O)CCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	298.42

Physical Properties

Property code	Value	Unit	Source
gf	-302.68	kJ/mol	Joback Method
hf	-782.43	kJ/mol	Joback Method
hfus	34.99	kJ/mol	Joback Method
hvap	70.54	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.032		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	1856.00		NIST Webbook
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tb	743.78	K	Joback Method
tc	930.72	K	Joback Method
tf	375.59	K	Joback Method
vc	0.998	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.78	J/molxK	743.78	Joback Method
cpg	844.87	J/molxK	899.56	Joback Method
cpg	831.44	J/molxK	868.41	Joback Method
cpg	817.13	J/molxK	837.25	Joback Method
cpg	801.94	J/molxK	806.09	Joback Method
cpg	785.82	J/molxK	774.94	Joback Method
cpg	857.44	J/molxK	930.72	Joback Method
dvisc	0.0000550	Paxs	743.78	Joback Method

dvisc	0.0000766	Paxs	682.41	Joback Method
dvisc	0.0001138	Paxs	621.05	Joback Method
dvisc	0.0001846	Paxs	559.68	Joback Method
dvisc	0.0003371	Paxs	498.32	Joback Method
dvisc	0.0007291	Paxs	436.96	Joback Method
dvisc	0.0020291	Paxs	375.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U391021&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

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