

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

Inchi:	InChI=1S/C18H32O4/c1-6-9-10-11-15(7-2)21-17(19)12-13-18(20)22-16(8-3)14(4)5/h7,14
InchiKey:	XCEAABHQAFXQIU-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	C=CC(CCCCC)OC(=O)CCC(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-286.64	kJ/mol	Joback Method
hf	-794.86	kJ/mol	Joback Method
hfus	36.10	kJ/mol	Joback Method
hvap	72.14	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.423		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
tb	759.18	K	Joback Method
tc	943.63	K	Joback Method
tf	390.18	K	Joback Method
vc	1.054	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.17	J/mol×K	759.18	Joback Method
cpg	842.53	J/mol×K	789.92	Joback Method
cpg	858.93	J/mol×K	820.66	Joback Method
cpg	874.38	J/mol×K	851.41	Joback Method
cpg	888.88	J/mol×K	882.15	Joback Method
cpg	902.47	J/mol×K	912.89	Joback Method
cpg	915.15	J/mol×K	943.63	Joback Method
dvisc	0.0018969	Paxs	390.18	Joback Method

dvisc	0.0007164	Paxs	451.68	Joback Method
dvisc	0.0003417	Paxs	513.18	Joback Method
dvisc	0.0001910	Paxs	574.68	Joback Method
dvisc	0.0001194	Paxs	636.18	Joback Method
dvisc	0.0000811	Paxs	697.68	Joback Method
dvisc	0.0000587	Paxs	759.18	Joback Method

Sources

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=U391318&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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