Succinic acid, hept-2-yl pent-4-en-2-yl ester

Inchi: InChI=1S/C16H28O4/c1-5-7-8-10-14(4)20-16(18)12-11-15(17)19-13(3)9-6-2/h6,13-14H,2
InchiKey: ZDBPPVSRRZUSCK-UHFFFAOYSA-N
Formula: C16H28O4
SMILES: C=CCC(C)OC(=O)CCC(=O)OC(C)CCCCC
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-301.04	kJ/mol	Joback Method
hf	-748.30	kJ/mol	Joback Method
hfus	34.44	kJ/mol	Joback Method
hvap	68.08	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.786		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1763.00		NIST Webbook
tb	713.86	K	Joback Method
tc	895.86	K	Joback Method
tf	382.64	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.01	J/mol×K	713.86	Joback Method
cpg	783.88	J/mol×K	865.53	Joback Method
cpg	770.77	J/mol×K	835.20	Joback Method
cpg	756.84	J/mol×K	804.86	Joback Method
cpg	742.08	J/mol×K	774.53	Joback Method
cpg	726.47	J/mol×K	744.19	Joback Method
cpg	796.17	J/mol×K	895.86	Joback Method
dvisc	0.0000837	Pa×s	713.86	Joback Method

dvisc	0.0001130	Pa×s	658.66	Joback Method
dvisc	0.0001614	Pa×s	603.45	Joback Method
dvisc	0.0002476	Pa×s	548.25	Joback Method
dvisc	0.0004179	Pa×s	493.05	Joback Method
dvisc	0.0008051	Pa×s	437.84	Joback Method
dvisc	0.0018739	Pa×s	382.64	Joback Method

Sources

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=U391157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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