Succinic acid, 2-methylpent-3-yl hept-1,6-dien-4-yl ester

Inchi: InChI=1S/C17H28O4/c1-6-9-14(10-7-2)20-16(18)11-12-17(19)21-15(8-3)13(4)5/h6-7,13-

InchiKey: BTCMHWDKOYUBSN-UHFFFAOYSA-N

Formula: C17H28O4

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

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-207.22	kJ/mol	Joback Method
hf	-648.79	kJ/mol	Joback Method
hfus	32.23	kJ/mol	Joback Method
hvap	69.24	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.808		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	1808.00		NIST Webbook
rinpol	1808.00		NIST Webbook
tb	732.98	K	Joback Method
tc	918.95	K	Joback Method
tf	377.15	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.29	J/mol×K	732.98	Joback Method
cpg	758.83	J/mol×K	763.98	Joback Method
cpg	774.44	J/mol×K	794.97	Joback Method
cpg	789.17	J/mol×K	825.97	Joback Method
cpg	803.01	J/mol×K	856.96	Joback Method
cpg	815.99	J/mol×K	887.96	Joback Method
cpg	828.13	J/mol×K	918.95	Joback Method
dvisc	0.0021130	Pa×s	377.15	Joback Method

dvisc	0.0008190	Pa×s	436.45	Joback Method
dvisc	0.0003982	Pa×s	495.76	Joback Method
dvisc	0.0002259	Pa×s	555.07	Joback Method
dvisc	0.0001429	Pa×s	614.37	Joback Method
dvisc	0.0000981	Pa×s	673.67	Joback Method
dvisc	0.0000715	Pa×s	732.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391330&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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