Succinic acid, hept-2-yl (2-methylcyclohex-1-en-1-yl)methyl ester

Inchi: InChI=1S/C19H32O4/c1-4-5-6-10-16(3)23-19(21)13-12-18(20)22-14-17-11-8-7-9-15(17)2

InchiKey: SCAYWPZKXOXFEK-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)OCC1=C(C)CCCC1

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-318.32	kJ/mol	Joback Method
hf	-820.87	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.712		Crippen Method
mcvol	278.290	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook
tb	819.60	K	Joback Method
tc	1019.44	K	Joback Method
tf	470.63	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.94	J/mol×K	819.60	Joback Method
cpg	892.55	J/mol×K	852.91	Joback Method
cpg	908.95	J/mol×K	886.21	Joback Method
cpg	924.17	J/mol×K	919.52	Joback Method
cpg	938.22	J/mol×K	952.83	Joback Method
cpg	951.13	J/mol×K	986.13	Joback Method
cpg	962.90	J/mol×K	1019.44	Joback Method
dvisc	0.0007869	Pa×s	470.63	Joback Method

dvisc	0.0003860	Pa×s	528.79	Joback Method
dvisc	0.0002181	Pa×s	586.95	Joback Method
dvisc	0.0001366	Pa×s	645.12	Joback Method
dvisc	0.0000924	Pa×s	703.28	Joback Method
dvisc	0.0000664	Pa×s	761.44	Joback Method
dvisc	0.0000499	Pa×s	819.60	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=U391417&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