Succinic acid, 2-methylpent-3-yl 1-phenylpropyl ester

Inchi: InChI=1S/C19H28O4/c1-5-16(14(3)4)22-18(20)12-13-19(21)23-17(6-2)15-10-8-7-9-11-15

InchiKey: RMJVNRLHXFKBEC-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CCC(OC(=O)CCC(=O)OC(CC)C(C)C)c1ccccc1

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-253.65	kJ/mol	Joback Method
hf	-704.40	kJ/mol	Joback Method
hfus	34.01	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.439		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
tb	812.06	K	Joback Method
tc	1017.36	K	Joback Method
tf	429.63	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.29	J/mol×K	812.06	Joback Method
cpg	837.81	J/mol×K	846.28	Joback Method
cpg	853.13	J/mol×K	880.49	Joback Method
cpg	867.29	J/mol×K	914.71	Joback Method
cpg	880.31	J/mol×K	948.93	Joback Method
cpg	892.22	J/mol×K	983.15	Joback Method
cpg	903.04	J/mol×K	1017.36	Joback Method
dvisc	0.0012680	Pa×s	429.63	Joback Method
dvisc	0.0005171	Pa×s	493.37	Joback Method
dvisc	0.0002589	Pa×s	557.11	Joback Method

dvisc	0.0001494	Pa×s	620.85	Joback Method
dvisc	0.0000955	Pa×s	684.58	Joback Method
dvisc	0.0000659	Pa×s	748.32	Joback Method
dvisc	0.0000482	Pa×s	812.06	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=U389924&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume