Succinic acid, 3-methylbut-2-en-1-yl 1-phenylpropyl ester

Inchi: InChI=1S/C18H24O4/c1-4-16(15-8-6-5-7-9-15)22-18(20)11-10-17(19)21-13-12-14(2)3/h5

InchiKey: AAIBGICLDSKGCK-UHFFFAOYSA-N

Formula: C18H24O4

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

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-185.52	kJ/mol	Joback Method
hf	-565.77	kJ/mol	Joback Method
hfus	37.36	kJ/mol	Joback Method
hvap	75.90	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.970		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
tb	794.10	K	Joback Method
tc	1003.13	K	Joback Method
tf	429.32	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.74	J/mol×K	794.10	Joback Method
cpg	752.37	J/mol×K	828.94	Joback Method
cpg	766.92	J/mol×K	863.78	Joback Method
cpg	780.43	J/mol×K	898.62	Joback Method
cpg	792.93	J/mol×K	933.45	Joback Method
cpg	804.47	J/mol×K	968.29	Joback Method
cpg	815.08	J/mol×K	1003.13	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=U389925&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
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