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

Inchi: InChI=1S/C18H24O5/c1-13(2)11-12-21-17(19)9-10-18(20)23-16-8-6-5-7-15(16)22-14(3)4

InchiKey: PQBMVRLCQWQQAB-UHFFFAOYSA-N

Formula: C18H24O5

SMILES: CC(C)=CCOC(=O)CCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-300.15	kJ/mol	Joback Method
hf	-709.46	kJ/mol	Joback Method
hfus	38.16	kJ/mol	Joback Method
hvap	78.97	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.669		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	821.50	K	Joback Method
tc	1030.69	K	Joback Method
tf	464.07	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.11	J/mol×K	821.50	Joback Method
cpg	779.17	J/mol×K	856.37	Joback Method
cpg	793.11	J/mol×K	891.23	Joback Method
cpg	805.95	J/mol×K	926.10	Joback Method
cpg	817.71	J/mol×K	960.96	Joback Method
cpg	828.41	J/mol×K	995.83	Joback Method
cpg	838.07	J/mol×K	1030.69	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389789&Units=SI

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