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

Inchi: InChI=1S/C18H26O5/c1-12(2)14(5)22-17(19)10-11-18(20)23-16-9-7-6-8-15(16)21-13(3)4

InchiKey: NGLCUALXIUIYSH-UHFFFAOYSA-N

Formula: C18H26O5

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

Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-376.70	kJ/mol	Joback Method
hf	-827.45	kJ/mol	Joback Method
hfus	32.22	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.747		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	816.58	K	Joback Method
tc	1023.31	K	Joback Method
tf	453.11	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.62	J/mol×K	816.58	Joback Method
cpg	807.35	J/mol×K	851.03	Joback Method
cpg	821.88	J/mol×K	885.49	Joback Method
cpg	835.21	J/mol×K	919.94	Joback Method
cpg	847.33	J/mol×K	954.40	Joback Method
cpg	858.27	J/mol×K	988.85	Joback Method
cpg	868.01	J/mol×K	1023.31	Joback Method
dvisc	0.0007705	Pa×s	453.11	Joback Method

dvisc	0.0003567	Pa×s	513.69	Joback Method
dvisc	0.0001942	Pa×s	574.27	Joback Method
dvisc	0.0001188	Pa×s	634.85	Joback Method
dvisc	0.0000791	Pa×s	695.42	Joback Method
dvisc	0.0000563	Pa×s	756.00	Joback Method
dvisc	0.0000421	Pa×s	816.58	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=U389787&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
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