Succinic acid, 3,4-dimethylphenyl 4-isopropylphenyl ester

Inchi: InChI=1S/C21H24O4/c1-14(2)17-6-9-18(10-7-17)24-20(22)11-12-21(23)25-19-8-5-15(3)16(4)13-19/h5-10,13-14H,11-12H2,1-4H3

InchiKey: NUFQEKQPDFLMDB-UHFFFAOYSA-N

Formula: C21H24O4

SMILES: Cc1ccc(OC(=O)CCC(=O)Oc2ccc(C(C)C)cc2)cc1C

Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-148.41	kJ/mol	Joback Method
hf	-533.00	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.718		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	2737.00		NIST Webbook
tb	900.32	K	Joback Method
tc	1126.79	K	Joback Method
tf	546.15	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.63	J/mol×K	900.32	Joback Method
cpg	895.17	J/mol×K	1089.05	Joback Method
cpg	886.28	J/mol×K	1051.30	Joback Method
cpg	876.11	J/mol×K	1013.56	Joback Method
cpg	864.63	J/mol×K	975.81	Joback Method
cpg	851.81	J/mol×K	938.07	Joback Method
cpg	902.81	J/mol×K	1126.79	Joback Method
dvisc	0.0000463	Pa×s	900.32	Joback Method
dvisc	0.0000584	Pa×s	841.29	Joback Method

dvisc	0.0000763	Pa×s	782.26	Joback Method
dvisc	0.0001040	Pa×s	723.23	Joback Method
dvisc	0.0001499	Pa×s	664.21	Joback Method
dvisc	0.0002321	Pa×s	605.18	Joback Method
dvisc	0.0003948	Pa×s	546.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360721&Units=SI
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

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