Succinic acid, 2-methylpent-3-yl 4-acetylphenyl ester

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

InchiKey: DVGOCDNQHIITKD-UHFFFAOYSA-N

Formula: C18H24O5

SMILES: CCC(OC(=O)CCC(=O)Oc1ccc(C(C)=O)cc1)C(C)C

Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-398.18	kJ/mol	Joback Method
hf	-802.53	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.553		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2417.00		NIST Webbook
rinpol	2417.00		NIST Webbook
tb	848.47	K	Joback Method
tc	1059.89	K	Joback Method
tf	495.81	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.72	J/mol×K	848.47	Joback Method
cpg	792.92	J/mol×K	883.71	Joback Method
cpg	805.94	J/mol×K	918.94	Joback Method
cpg	817.81	J/mol×K	954.18	Joback Method
cpg	828.53	J/mol×K	989.42	Joback Method
cpg	838.13	J/mol×K	1024.66	Joback Method
cpg	846.63	J/mol×K	1059.89	Joback Method
dvisc	0.0007509	Pa×s	495.81	Joback Method

dvisc	0.0003916	Pa×s	554.59	Joback Method
dvisc	0.0002313	Pa×s	613.36	Joback Method
dvisc	0.0001498	Pa×s	672.14	Joback Method
dvisc	0.0001041	Pa×s	730.92	Joback Method
dvisc	0.0000763	Pa×s	789.69	Joback Method
dvisc	0.0000584	Pa×s	848.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389910&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