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

Inchi: InChI=1S/C17H22O5/c1-11(2)13(4)21-16(19)9-10-17(20)22-15-7-5-14(6-8-15)12(3)18/h5
InchiKey: SAYBTAKJMVDACF-UHFFFAOYSA-N
Formula: C17H22O5
SMILES: CC(=O)c1ccc(OC(=O)CCC(=O)OC(C)C(C)C)cc1
Mol. weight [g/mol]: 306.35

Physical Properties

Property code	Value	Unit	Source
gf	-406.60	kJ/mol	Joback Method
hf	-781.89	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.163		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2334.00		NIST Webbook
rinpol	2334.00		NIST Webbook
tb	825.59	K	Joback Method
tc	1038.03	K	Joback Method
tf	484.54	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.72	J/mol×K	825.59	Joback Method
cpg	735.75	J/mol×K	861.00	Joback Method
cpg	748.64	J/mol×K	896.40	Joback Method
cpg	760.40	J/mol×K	931.81	Joback Method
cpg	771.05	J/mol×K	967.22	Joback Method
cpg	780.61	J/mol×K	1002.62	Joback Method
cpg	789.09	J/mol×K	1038.03	Joback Method
dvisc	0.0008322	Pa×s	484.54	Joback Method

dvisc	0.0004390	Pa×s	541.38	Joback Method
dvisc	0.0002615	Pa×s	598.22	Joback Method
dvisc	0.0001704	Pa×s	655.06	Joback Method
dvisc	0.0001189	Pa×s	711.91	Joback Method
dvisc	0.0000875	Pa×s	768.75	Joback Method
dvisc	0.0000672	Pa×s	825.59	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=U389909&Units=SI

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