Sebacic acid, 4-acetylphenyl butyl ester

Inchi: InChI=1S/C22H32O5/c1-3-4-17-26-21(24)11-9-7-5-6-8-10-12-22(25)27-20-15-13-19(14-1
InchiKey: UQBUNXCADRGERN-UHFFFAOYSA-N
Formula: C22H32O5
SMILES: CCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 376.49

Physical Properties

Property code	Value	Unit	Source
gf	-359.62	kJ/mol	Joback Method
hf	-874.53	kJ/mol	Joback Method
hfus	53.56	kJ/mol	Joback Method
hvap	92.56	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.259		Crippen Method
mcvol	313.530	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpol	3017.00		NIST Webbook
rinpol	3017.00		NIST Webbook
tb	940.87	K	Joback Method
tc	1153.86	K	Joback Method
tf	570.89	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.10	J/mol×K	940.87	Joback Method
cpg	1027.78	J/mol×K	976.37	Joback Method
cpg	1041.14	J/mol×K	1011.87	Joback Method
cpg	1053.22	J/mol×K	1047.37	Joback Method
cpg	1064.04	J/mol×K	1082.87	Joback Method
cpg	1073.62	J/mol×K	1118.37	Joback Method
cpg	1082.02	J/mol×K	1153.86	Joback Method
dvisc	0.0003931	Pa×s	570.89	Joback Method

dvisc	0.0002220	Pa×s	632.55	Joback Method
dvisc	0.0001387	Pa×s	694.22	Joback Method
dvisc	0.0000936	Pa×s	755.88	Joback Method
dvisc	0.0000670	Pa×s	817.54	Joback Method
dvisc	0.0000503	Pa×s	879.21	Joback Method
dvisc	0.0000392	Pa×s	940.87	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=U354963&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