Sebacic acid, 4-acetylphenyl nonyl ester

Inchi: InChI=1S/C27H42O5/c1-3-4-5-6-9-12-15-22-31-26(29)16-13-10-7-8-11-14-17-27(30)32-2
InchiKey: XEMOGXSSPLVLTM-UHFFFAOYSA-N
Formula: C27H42O5
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 446.62

Physical Properties

Property code	Value	Unit	Source
gf	-317.52	kJ/mol	Joback Method
hf	-977.73	kJ/mol	Joback Method
hfus	66.51	kJ/mol	Joback Method
hvap	103.69	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.209		Crippen Method
mcvol	383.980	ml/mol	McGowan Method
pc	896.95	kPa	Joback Method
rinpol	3545.00		NIST Webbook
rinpol	3545.00		NIST Webbook
tb	1055.27	K	Joback Method
tc	1297.12	K	Joback Method
tf	627.24	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.47	J/mol×K	1055.27	Joback Method
cpg	1335.23	J/mol×K	1095.58	Joback Method
cpg	1349.17	J/mol×K	1135.89	Joback Method
cpg	1361.37	J/mol×K	1176.20	Joback Method
cpg	1371.88	J/mol×K	1216.51	Joback Method
cpg	1380.78	J/mol×K	1256.82	Joback Method
cpg	1388.14	J/mol×K	1297.12	Joback Method
dvisc	0.0002157	Pa×s	627.24	Joback Method

dvisc	0.0001158	Pa×s	698.58	Joback Method
dvisc	0.0000698	Pa×s	769.92	Joback Method
dvisc	0.0000458	Pa×s	841.25	Joback Method
dvisc	0.0000322	Pa×s	912.59	Joback Method
dvisc	0.0000237	Pa×s	983.93	Joback Method
dvisc	0.0000183	Pa×s	1055.27	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=U354969&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