Sebacic acid, ethyl 4-(2-phenylpropyl-2)-phenyl ester

Inchi: InChI=1S/C27H36O4/c1-4-30-25(28)16-12-7-5-6-8-13-17-26(29)31-24-20-18-23(19-21-2
InchiKey: QHPZNIPVUYSUMW-UHFFFAOYSA-N
Formula: C27H36O4
SMILES: CCOC(=O)CCCCCCCCC(=O)Oc1ccc(C(C)(C)c2ccccc2)cc1
Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-73.35	kJ/mol	Joback Method
hf	-637.37	kJ/mol	Joback Method
hfus	51.54	kJ/mol	Joback Method
hvap	97.93	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.602		Crippen Method
mcvol	358.650	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	3346.00		NIST Webbook
tb	1024.85	K	Joback Method
tc	1256.82	K	Joback Method
tf	606.15	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.09	J/mol×K	1024.85	Joback Method
cpg	1214.06	J/mol×K	1063.51	Joback Method
cpg	1227.66	J/mol×K	1102.17	Joback Method
cpg	1239.99	J/mol×K	1140.84	Joback Method
cpg	1251.15	J/mol×K	1179.50	Joback Method
cpg	1261.23	J/mol×K	1218.16	Joback Method
cpg	1270.33	J/mol×K	1256.82	Joback Method
dvisc	0.0002031	Pa×s	606.15	Joback Method
dvisc	0.0001055	Pa×s	675.93	Joback Method

dvisc	0.0000619	Pa×s	745.72	Joback Method
dvisc	0.0000398	Pa×s	815.50	Joback Method
dvisc	0.0000275	Pa×s	885.28	Joback Method
dvisc	0.0000200	Pa×s	955.07	Joback Method
dvisc	0.0000152	Pa×s	1024.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354542&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

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