Sebacic acid, 2,6-dimethoxyphenyl nonyl ester

Inchi: InChI=1S/C27H44O6/c1-4-5-6-7-10-13-16-22-32-25(28)20-14-11-8-9-12-15-21-26(29)33
InchiKey: IBVLYWGLRVLUIH-UHFFFAOYSA-N
Formula: C27H44O6
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 464.63

Physical Properties

Property code	Value	Unit	Source
gf	-408.23	kJ/mol	Joback Method
hf	-1141.06	kJ/mol	Joback Method
hfus	66.90	kJ/mol	Joback Method
hvap	102.43	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.024		Crippen Method
mcvol	394.150	ml/mol	McGowan Method
pc	839.67	kPa	Joback Method
rinpol	3456.00		NIST Webbook
rinpol	3456.00		NIST Webbook
tb	1051.22	K	Joback Method
tc	1295.42	K	Joback Method
tf	634.29	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1362.75	J/mol×K	1051.22	Joback Method
cpg	1417.98	J/mol×K	1254.72	Joback Method
cpg	1411.51	J/mol×K	1214.02	Joback Method
cpg	1402.77	J/mol×K	1173.32	Joback Method
cpg	1391.74	J/mol×K	1132.62	Joback Method
cpg	1378.41	J/mol×K	1091.92	Joback Method
cpg	1422.21	J/mol×K	1295.42	Joback Method
dvisc	0.0000108	Pa×s	1051.22	Joback Method

dvisc	0.0000139	Pa×s	981.73	Joback Method
dvisc	0.0000187	Pa×s	912.24	Joback Method
dvisc	0.0000262	Pa×s	842.75	Joback Method
dvisc	0.0000392	Pa×s	773.27	Joback Method
dvisc	0.0000633	Pa×s	703.78	Joback Method
dvisc	0.0001138	Pa×s	634.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354757&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