Sebacic acid, di(2,6-dimethoxyphenyl) ester

Inchi: InChI=1S/C26H34O8/c1-29-19-13-11-14-20(30-2)25(19)33-23(27)17-9-7-5-6-8-10-18-24(28)34-26-21(31-3)15-12-16-22(26)32-4

InchiKey: PLSUQFFUSMXNBZ-UHFFFAOYSA-N

Formula: C26H34O8

SMILES: COc1cccc(OC)c1OC(=O)CCCCCCCCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 474.54

Physical Properties

Property code	Value	Unit	Source
gf	-533.50	kJ/mol	Joback Method
hf	-1171.27	kJ/mol	Joback Method
hfus	59.95	kJ/mol	Joback Method
hvap	108.62	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.353		Crippen Method
mcvol	368.040	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	3324.00		NIST Webbook
tb	1109.82	K	Joback Method
tc	1361.00	K	Joback Method
tf	718.94	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1233.69	J/mol×K	1109.82	Joback Method
cpg	1241.26	J/mol×K	1151.68	Joback Method
cpg	1245.97	J/mol×K	1193.55	Joback Method
cpg	1247.77	J/mol×K	1235.41	Joback Method
cpg	1246.62	J/mol×K	1277.27	Joback Method
cpg	1242.47	J/mol×K	1319.14	Joback Method
cpg	1235.29	J/mol×K	1361.00	Joback Method
dvisc	0.0000494	Pa×s	718.94	Joback Method
dvisc	0.0000317	Pa×s	784.09	Joback Method

dvisc	0.0000218	Pa×s	849.23	Joback Method
dvisc	0.0000158	Pa×s	914.38	Joback Method
dvisc	0.0000119	Pa×s	979.53	Joback Method
dvisc	0.0000093	Pa×s	1044.67	Joback Method
dvisc	0.0000075	Pa×s	1109.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354761&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