Sebacic acid, 2,6-dimethoxyphenyl octyl ester

Inchi: InChI=1S/C26H42O6/c1-4-5-6-7-12-15-21-31-24(27)19-13-10-8-9-11-14-20-25(28)32-26
InchiKey: SHEROTSNYLCYAV-UHFFFAOYSA-N
Formula: C26H42O6
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 450.61

Physical Properties

Property code	Value	Unit	Source
gf	-416.65	kJ/mol	Joback Method
hf	-1120.42	kJ/mol	Joback Method
hfus	64.31	kJ/mol	Joback Method
hvap	100.20	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.634		Crippen Method
mcvol	380.060	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	3354.00		NIST Webbook
rinpol	3354.00		NIST Webbook
tb	1028.34	K	Joback Method
tc	1263.49	K	Joback Method
tf	623.02	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.73	J/mol×K	1028.34	Joback Method
cpg	1316.32	J/mol×K	1067.53	Joback Method
cpg	1329.80	J/mol×K	1106.72	Joback Method
cpg	1341.17	J/mol×K	1145.91	Joback Method
cpg	1350.45	J/mol×K	1185.10	Joback Method
cpg	1357.66	J/mol×K	1224.30	Joback Method
cpg	1362.80	J/mol×K	1263.49	Joback Method
dvisc	0.0001289	Pa×s	623.02	Joback Method

dvisc	0.0000725	Pa×s	690.57	Joback Method
dvisc	0.0000451	Pa×s	758.13	Joback Method
dvisc	0.0000304	Pa×s	825.68	Joback Method
dvisc	0.0000217	Pa×s	893.23	Joback Method
dvisc	0.0000163	Pa×s	960.79	Joback Method
dvisc	0.0000126	Pa×s	1028.34	Joback Method

Sources

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=U354756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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