Fumaric acid, 3,4-dimethoxyphenyl pentadecyl ester

Inchi: InChI=1S/C27H42O6/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-21-32-26(28)19-20-27(29)33

InchiKey: ONRBYRMPPLMOJB-FMQUCBEESA-N

Formula: C27H42O6

SMILES: CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)Oc1ccc(OC)c(OC)c1

Mol. weight [g/mol]: 462.62

Physical Properties

Property code	Value	Unit	Source
gf	-328.01	kJ/mol	Joback Method
hf	-1023.84	kJ/mol	Joback Method
hfus	67.10	kJ/mol	Joback Method
hvap	102.39	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.800		Crippen Method
mcvol	389.850	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpol	3507.00		NIST Webbook
rinpol	3507.00		NIST Webbook
tb	1055.38	K	Joback Method
tc	1297.97	K	Joback Method
tf	629.21	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1333.77	J/mol×K	1055.38	Joback Method
cpg	1391.06	J/mol×K	1257.54	Joback Method
cpg	1383.56	J/mol×K	1217.11	Joback Method
cpg	1374.12	J/mol×K	1176.68	Joback Method
cpg	1362.70	J/mol×K	1136.24	Joback Method
cpg	1349.26	J/mol×K	1095.81	Joback Method
cpg	1396.65	J/mol×K	1297.97	Joback Method
dvisc	0.0000095	Pa×s	1055.38	Joback Method

dvisc	0.0000123	Pa×s	984.35	Joback Method
dvisc	0.0000165	Pa×s	913.32	Joback Method
dvisc	0.0000233	Pa×s	842.29	Joback Method
dvisc	0.0000351	Pa×s	771.27	Joback Method
dvisc	0.0000575	Pa×s	700.24	Joback Method
dvisc	0.0001050	Pa×s	629.21	Joback Method

Sources

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=U348176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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