Fumaric acid, 3,4-dimethoxyphenyl undecyl ester

Inchi: InChI=1S/C23H34O6/c1-4-5-6-7-8-9-10-11-12-17-28-22(24)15-16-23(25)29-19-13-14-20

InchiKey: ZAIFUMROOCZVLN-FOCLMDBBSA-N

Formula: C23H34O6

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

Mol. weight [g/mol]: 406.51

Physical Properties

Property code	Value	Unit	Source
gf	-361.69	kJ/mol	Joback Method
hf	-941.28	kJ/mol	Joback Method
hfus	56.74	kJ/mol	Joback Method
hvap	93.48	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.239		Crippen Method
mcvol	333.490	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	3101.00		NIST Webbook
tb	963.86	K	Joback Method
tc	1180.35	K	Joback Method
tf	584.13	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.79	J/mol×K	963.86	Joback Method
cpg	1147.54	J/mol×K	1144.27	Joback Method
cpg	1138.57	J/mol×K	1108.18	Joback Method
cpg	1128.12	J/mol×K	1072.10	Joback Method
cpg	1116.18	J/mol×K	1036.02	Joback Method
cpg	1102.75	J/mol×K	999.94	Joback Method
cpg	1155.05	J/mol×K	1180.35	Joback Method
dvisc	0.0000176	Pa×s	963.86	Joback Method
dvisc	0.0000225	Pa×s	900.57	Joback Method

dvisc	0.0000298	Pa×s	837.28	Joback Method
dvisc	0.0000414	Pa×s	773.99	Joback Method
dvisc	0.0000609	Pa×s	710.71	Joback Method
dvisc	0.0000968	Pa×s	647.42	Joback Method
dvisc	0.0001699	Pa×s	584.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348174&Units=SI

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