Fumaric acid, 3,4-dimethoxyphenyl pentyl ester

Inchi: InChI=1S/C17H22O6/c1-4-5-6-11-22-16(18)9-10-17(19)23-13-7-8-14(20-2)15(12-13)21-3

InchiKey: ZPJSIRPMCHFOFI-MDZDMXLPSA-N

Formula: C17H22O6

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

Mol. weight [g/mol]: 322.35

Physical Properties

Property code	Value	Unit	Source
gf	-412.21	kJ/mol	Joback Method
hf	-817.44	kJ/mol	Joback Method
hfus	41.20	kJ/mol	Joback Method
hvap	80.13	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.899		Crippen Method
mcvol	248.950	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	826.58	K	Joback Method
tc	1032.71	K	Joback Method
tf	516.51	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.80	J/mol×K	826.58	Joback Method
cpg	747.78	J/mol×K	860.94	Joback Method
cpg	760.68	J/mol×K	895.29	Joback Method
cpg	772.48	J/mol×K	929.65	Joback Method
cpg	783.19	J/mol×K	964.00	Joback Method
cpg	792.79	J/mol×K	998.36	Joback Method
cpg	801.29	J/mol×K	1032.71	Joback Method
dvisc	0.0003165	Pa×s	516.51	Joback Method

dvisc	0.0001933	Pa×s	568.19	Joback Method
dvisc	0.0001282	Pa×s	619.87	Joback Method
dvisc	0.0000906	Pa×s	671.54	Joback Method
dvisc	0.0000672	Pa×s	723.22	Joback Method
dvisc	0.0000520	Pa×s	774.90	Joback Method
dvisc	0.0000414	Pa×s	826.58	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=U348167&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