Fumaric acid, 3,4-dimethoxyphenyl nonyl ester

Inchi: InChI=1S/C21H30O6/c1-4-5-6-7-8-9-10-15-26-20(22)13-14-21(23)27-17-11-12-18(24-2)1

InchiKey: KXFMBMCMVYNTBU-BUHFOSPRSA-N

Formula: C21H30O6

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

Mol. weight [g/mol]: 378.46

Physical Properties

Property code	Value	Unit	Source
gf	-378.53	kJ/mol	Joback Method
hf	-900.00	kJ/mol	Joback Method
hfus	51.56	kJ/mol	Joback Method
hvap	89.03	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.459		Crippen Method
mcvol	305.310	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	2884.00		NIST Webbook
rinpol	2884.00		NIST Webbook
tb	918.10	K	Joback Method
tc	1127.82	K	Joback Method
tf	561.59	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.30	J/mol×K	918.10	Joback Method
cpg	1027.37	J/mol×K	1092.86	Joback Method
cpg	1018.01	J/mol×K	1057.91	Joback Method
cpg	1007.32	J/mol×K	1022.96	Joback Method
cpg	995.32	J/mol×K	988.01	Joback Method
cpg	981.98	J/mol×K	953.05	Joback Method
cpg	1035.41	J/mol×K	1127.82	Joback Method
dvisc	0.0000236	Pa×s	918.10	Joback Method

dvisc	0.0000300	Pa×s	858.68	Joback Method
dvisc	0.0000395	Pa×s	799.26	Joback Method
dvisc	0.0000543	Pa×s	739.84	Joback Method
dvisc	0.0000790	Pa×s	680.43	Joback Method
dvisc	0.0001235	Pa×s	621.01	Joback Method
dvisc	0.0002122	Pa×s	561.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348172&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