Fumaric acid, 2,6-dimethoxyphenyl 3-methylbut-2-yl ester

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

InchiKey: HHMNGYFMAWSUTA-MDZDMXLPSA-N

Formula: C17H22O6

SMILES: COc1cccc(OC)c1OC(=O)C=CC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 322.35

Physical Properties

Property code	Value	Unit	Source
gf	-417.09	kJ/mol	Joback Method
hf	-828.00	kJ/mol	Joback Method
hfus	34.16	kJ/mol	Joback Method
hvap	79.35	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.753		Crippen Method
mcvol	248.950	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	825.70	K	Joback Method
tc	1036.73	K	Joback Method
tf	486.51	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.91	J/mol×K	825.70	Joback Method
cpg	749.21	J/mol×K	860.87	Joback Method
cpg	762.34	J/mol×K	896.04	Joback Method
cpg	774.30	J/mol×K	931.22	Joback Method
cpg	785.09	J/mol×K	966.39	Joback Method
cpg	794.70	J/mol×K	1001.56	Joback Method
cpg	803.13	J/mol×K	1036.73	Joback Method
dvisc	0.0003950	Pa×s	486.51	Joback Method

dvisc	0.0002135	Pa×s	543.04	Joback Method
dvisc	0.0001296	Pa×s	599.57	Joback Method
dvisc	0.0000858	Pa×s	656.11	Joback Method
dvisc	0.0000606	Pa×s	712.64	Joback Method
dvisc	0.0000450	Pa×s	769.17	Joback Method
dvisc	0.0000349	Pa×s	825.70	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=U405749&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