Fumaric acid, 2,6-dimethoxyphenyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C17H20O6/c1-12(2)10-11-22-15(18)8-9-16(19)23-17-13(20-3)6-5-7-14(17)21-4

InchiKey: BTVLEQBHNAPDFI-CMDGGOBGSA-N

Formula: C17H20O6

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

Mol. weight [g/mol]: 320.34

Physical Properties

Property code	Value	Unit	Source
gf	-340.54	kJ/mol	Joback Method
hf	-710.01	kJ/mol	Joback Method
hfus	40.09	kJ/mol	Joback Method
hvap	80.16	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.675		Crippen Method
mcvol	244.650	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2385.00		NIST Webbook
tb	830.62	K	Joback Method
tc	1044.20	K	Joback Method
tf	497.47	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.97	J/mol×K	830.62	Joback Method
cpg	720.59	J/mol×K	866.22	Joback Method
cpg	733.16	J/mol×K	901.81	Joback Method
cpg	744.67	J/mol×K	937.41	Joback Method
cpg	755.13	J/mol×K	973.01	Joback Method
cpg	764.55	J/mol×K	1008.60	Joback Method
cpg	772.94	J/mol×K	1044.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405751&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

Legend

cpg:	Ideal gas heat capacity
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