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

Inchi: InChI=1S/C18H24O6/c1-6-13(12(2)3)23-16(19)10-11-17(20)24-18-14(21-4)8-7-9-15(18)2

InchiKey: ZSTQLCUKIWOSAL-ZHACJKMWSA-N

Formula: C18H24O6

SMILES: CCC(OC(=O)C=CC(=O)Oc1c(OC)cccc1OC)C(C)C

Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	-408.67	kJ/mol	Joback Method
hf	-848.64	kJ/mol	Joback Method
hfus	36.74	kJ/mol	Joback Method
hvap	81.58	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.143		Crippen Method
mcvol	263.040	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook
tb	848.58	K	Joback Method
tc	1058.77	K	Joback Method
tf	497.78	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.15	J/mol×K	848.58	Joback Method
cpg	806.60	J/mol×K	883.61	Joback Method
cpg	819.84	J/mol×K	918.64	Joback Method
cpg	831.86	J/mol×K	953.67	Joback Method
cpg	842.67	J/mol×K	988.70	Joback Method
cpg	852.25	J/mol×K	1023.74	Joback Method
cpg	860.61	J/mol×K	1058.77	Joback Method
dvisc	0.0003571	Pa×s	497.78	Joback Method

dvisc	0.0001908	Pa×s	556.25	Joback Method
dvisc	0.0001148	Pa×s	614.71	Joback Method
dvisc	0.0000755	Pa×s	673.18	Joback Method
dvisc	0.0000531	Pa×s	731.65	Joback Method
dvisc	0.0000393	Pa×s	790.11	Joback Method
dvisc	0.0000303	Pa×s	848.58	Joback Method

Sources

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=U405750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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