Fumaric acid, butyl 3,4-dimethoxyphenyl ester

Inchi: InChI=1S/C16H20O6/c1-4-5-10-21-15(17)8-9-16(18)22-12-6-7-13(19-2)14(11-12)20-3/h6
InchiKey: PQYHMLFEDDSNHV-CMDGGOBGSA-N
Formula: C16H20O6
SMILES: CCCCOC(=O)C=CC(=O)Oc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 308.33

Physical Properties

Property code	Value	Unit	Source
gf	-420.63	kJ/mol	Joback Method
hf	-796.80	kJ/mol	Joback Method
hfus	38.61	kJ/mol	Joback Method
hvap	77.90	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.509		Crippen Method
mcvol	234.860	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2365.00		NIST Webbook
tb	803.70	K	Joback Method
tc	1010.69	K	Joback Method
tf	505.24	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.41	J/mol×K	803.70	Joback Method
cpg	735.66	J/mol×K	976.19	Joback Method
cpg	726.11	J/mol×K	941.70	Joback Method
cpg	715.51	J/mol×K	907.20	Joback Method
cpg	703.85	J/mol×K	872.70	Joback Method
cpg	691.14	J/mol×K	838.20	Joback Method
cpg	744.15	J/mol×K	1010.69	Joback Method
dvisc	0.0000474	Pa×s	803.70	Joback Method
dvisc	0.0000592	Pa×s	753.96	Joback Method

dvisc	0.0000762	Pa×s	704.21	Joback Method
dvisc	0.0001021	Pa×s	654.47	Joback Method
dvisc	0.0001434	Pa×s	604.73	Joback Method
dvisc	0.0002141	Pa×s	554.98	Joback Method
dvisc	0.0003460	Pa×s	505.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348166&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
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