Fumaric acid, ethyl 3,4-dimethoxyphenyl ester

Inchi: InChI=1S/C14H16O6/c1-4-19-13(15)7-8-14(16)20-10-5-6-11(17-2)12(9-10)18-3/h5-9H,4
InchiKey: UHIQRBXLMGNTQZ-BQYQJAHWSA-N
Formula: C14H16O6
SMILES: CCOC(=O)C=CC(=O)Oc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 280.27

Physical Properties

Property code	Value	Unit	Source
gf	-437.47	kJ/mol	Joback Method
hf	-755.52	kJ/mol	Joback Method
hfus	33.43	kJ/mol	Joback Method
hvap	73.45	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.728		Crippen Method
mcvol	206.680	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	2161.00		NIST Webbook
rinpol	2161.00		NIST Webbook
tb	757.94	K	Joback Method
tc	968.42	K	Joback Method
tf	482.70	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.56	J/mol×K	757.94	Joback Method
cpg	580.65	J/mol×K	793.02	Joback Method
cpg	592.80	J/mol×K	828.10	Joback Method
cpg	604.02	J/mol×K	863.18	Joback Method
cpg	614.27	J/mol×K	898.26	Joback Method
cpg	623.55	J/mol×K	933.34	Joback Method
cpg	631.85	J/mol×K	968.42	Joback Method
dvisc	0.0004070	Pa×s	482.70	Joback Method

dvisc	0.0002589	Pa×s	528.57	Joback Method
dvisc	0.0001770	Pa×s	574.45	Joback Method
dvisc	0.0001280	Pa×s	620.32	Joback Method
dvisc	0.0000968	Pa×s	666.19	Joback Method
dvisc	0.0000759	Pa×s	712.07	Joback Method
dvisc	0.0000613	Pa×s	757.94	Joback Method

Sources

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=U348163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/89-862-7/Fumaric-acid-ethyl-3-4-dimethoxyphenyl-ester.pdf
Generated by Cheméo on 2024-10-12 05:52:00.347559217 +0000 UTC m=+3293182.984528465.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.