Fumaric acid, 3,4-dimethoxyphenyl isobutyl ester

Inchi: InChI=1S/C16H20O6/c1-11(2)10-21-15(17)7-8-16(18)22-12-5-6-13(19-3)14(9-12)20-4/h5

InchiKey: IBYMUVVMUQFVHS-BQYQJAHWSA-N

Formula: C16H20O6

SMILES: COc1ccc(OC(=O)C=CC(=O)OCC(C)C)cc1OC

Mol. weight [g/mol]: 308.33

Physical Properties

Property code	Value	Unit	Source
gf	-423.07	kJ/mol	Joback Method
hf	-802.08	kJ/mol	Joback Method
hfus	35.09	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.365		Crippen Method
mcvol	234.860	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	2314.00		NIST Webbook
tb	803.26	K	Joback Method
tc	1012.94	K	Joback Method
tf	490.24	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.98	J/mol×K	803.26	Joback Method
cpg	736.71	J/mol×K	977.99	Joback Method
cpg	727.14	J/mol×K	943.05	Joback Method
cpg	716.48	J/mol×K	908.10	Joback Method
cpg	704.72	J/mol×K	873.15	Joback Method
cpg	691.88	J/mol×K	838.21	Joback Method
cpg	745.17	J/mol×K	1012.94	Joback Method
dvisc	0.0000435	Pa×s	803.26	Joback Method
dvisc	0.0000552	Pa×s	751.09	Joback Method

dvisc	0.0000724	Pa×s	698.92	Joback Method
dvisc	0.0000994	Pa×s	646.75	Joback Method
dvisc	0.0001442	Pa×s	594.58	Joback Method
dvisc	0.0002248	Pa×s	542.41	Joback Method
dvisc	0.0003850	Pa×s	490.24	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=U348165&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