Fumaric acid, 3,4-dimethoxyphenyl propyl ester

Inchi: InChI=1S/C15H18O6/c1-4-9-20-14(16)7-8-15(17)21-11-5-6-12(18-2)13(10-11)19-3/h5-8,

InchiKey: ZTJKSTVJDDCBPR-BQYQJAHWSA-N

Formula: C15H18O6

SMILES: CCCOC(=O)C=CC(=O)Oc1ccc(OC)c(OC)c1

Mol. weight [g/mol]: 294.30

Physical Properties

Property code	Value	Unit	Source
gf	-429.05	kJ/mol	Joback Method
hf	-776.16	kJ/mol	Joback Method
hfus	36.02	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.119		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	2253.00		NIST Webbook
tb	780.82	K	Joback Method
tc	989.28	K	Joback Method
tf	493.97	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.97	J/mol×K	780.82	Joback Method
cpg	635.41	J/mol×K	815.56	Joback Method
cpg	647.87	J/mol×K	850.31	Joback Method
cpg	659.33	J/mol×K	885.05	Joback Method
cpg	669.79	J/mol×K	919.79	Joback Method
cpg	679.24	J/mol×K	954.53	Joback Method
cpg	687.65	J/mol×K	989.28	Joback Method
dvisc	0.0003763	Pa×s	493.97	Joback Method
dvisc	0.0002360	Pa×s	541.78	Joback Method

dvisc	0.0001597	Pa×s	589.59	Joback Method
dvisc	0.0001146	Pa×s	637.39	Joback Method
dvisc	0.0000861	Pa×s	685.20	Joback Method
dvisc	0.0000671	Pa×s	733.01	Joback Method
dvisc	0.0000540	Pa×s	780.82	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=U348164&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

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