Fumaric acid, 4-methoxyphenyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C17H22O5/c1-5-15(12(2)3)22-17(19)11-10-16(18)21-14-8-6-13(20-4)7-9-14/h6

InchiKey: WRUHBWNRLWINNL-ZHACJKMWSA-N

Formula: C17H22O5

SMILES: CCC(OC(=O)C=CC(=O)Oc1ccc(OC)cc1)C(C)C

Mol. weight [g/mol]: 306.35

Physical Properties

Property code	Value	Unit	Source
gf	-302.46	kJ/mol	Joback Method
hf	-684.31	kJ/mol	Joback Method
hfus	33.36	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.135		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	798.30	K	Joback Method
tc	1009.29	K	Joback Method
tf	451.76	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.20	J/mol×K	798.30	Joback Method
cpg	723.09	J/mol×K	833.47	Joback Method
cpg	736.87	J/mol×K	868.63	Joback Method
cpg	749.56	J/mol×K	903.80	Joback Method
cpg	761.18	J/mol×K	938.96	Joback Method
cpg	771.74	J/mol×K	974.13	Joback Method
cpg	781.25	J/mol×K	1009.29	Joback Method
dvisc	0.0006771	Pa×s	451.76	Joback Method

dvisc	0.0003350	Pa×s	509.52	Joback Method
dvisc	0.0001913	Pa×s	567.27	Joback Method
dvisc	0.0001212	Pa×s	625.03	Joback Method
dvisc	0.0000829	Pa×s	682.79	Joback Method
dvisc	0.0000602	Pa×s	740.54	Joback Method
dvisc	0.0000458	Pa×s	798.30	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=U405778&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