Fumaric acid, 2-methoxyphenyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C16H20O5/c1-11(2)12(3)20-15(17)9-10-16(18)21-14-8-6-5-7-13(14)19-4/h5-12

InchiKey: ZXSHXGYSXHWSNC-MDZDMXLPSA-N

Formula: C16H20O5

SMILES: COc1ccccc1OC(=O)C=CC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 292.33

Physical Properties

Property code	Value	Unit	Source
gf	-310.88	kJ/mol	Joback Method
hf	-663.67	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	74.05	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.744		Crippen Method
mcvol	228.990	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2067.00		NIST Webbook
rinpol	2067.00		NIST Webbook
tb	775.42	K	Joback Method
tc	988.41	K	Joback Method
tf	440.49	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.33	J/mol×K	775.42	Joback Method
cpg	714.98	J/mol×K	952.91	Joback Method
cpg	704.54	J/mol×K	917.41	Joback Method
cpg	693.06	J/mol×K	881.91	Joback Method
cpg	680.55	J/mol×K	846.42	Joback Method
cpg	666.97	J/mol×K	810.92	Joback Method
cpg	724.39	J/mol×K	988.41	Joback Method
dvisc	0.0000523	Pa×s	775.42	Joback Method

dvisc	0.0000686	Pa×s	719.60	Joback Method
dvisc	0.0000942	Pa×s	663.78	Joback Method
dvisc	0.0001371	Pa×s	607.95	Joback Method
dvisc	0.0002151	Pa×s	552.13	Joback Method
dvisc	0.0003735	Pa×s	496.31	Joback Method
dvisc	0.0007462	Pa×s	440.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405928&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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