Fumaric acid, 2-methoxyphenyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C16H18O5/c1-12(2)10-11-20-15(17)8-9-16(18)21-14-7-5-4-6-13(14)19-3/h4-10

InchiKey: MNPHRLCACOUNFG-CMDGGOBGSA-N

Formula: C16H18O5

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

Mol. weight [g/mol]: 290.31

Physical Properties

Property code	Value	Unit	Source
gf	-234.33	kJ/mol	Joback Method
hf	-545.68	kJ/mol	Joback Method
hfus	36.70	kJ/mol	Joback Method
hvap	74.87	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.666		Crippen Method
mcvol	224.690	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	780.34	K	Joback Method
tc	996.25	K	Joback Method
tf	451.45	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.54	J/mol×K	780.34	Joback Method
cpg	639.39	J/mol×K	816.32	Joback Method
cpg	652.26	J/mol×K	852.31	Joback Method
cpg	664.17	J/mol×K	888.29	Joback Method
cpg	675.15	J/mol×K	924.28	Joback Method
cpg	685.22	J/mol×K	960.26	Joback Method
cpg	694.41	J/mol×K	996.25	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=U405930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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