Fumaric acid, 2-isopropoxyphenyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C19H26O5/c1-6-15(13(2)3)23-18(20)11-12-19(21)24-17-10-8-7-9-16(17)22-14

InchiKey: GMXKSHKITBRVFS-VAWYXSNFSA-N

Formula: C19H26O5

SMILES: CCC(OC(=O)C=CC(=O)Oc1ccccc1OC(C)C)C(C)C

Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-288.06	kJ/mol	Joback Method
hf	-730.87	kJ/mol	Joback Method
hfus	35.01	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.913		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
tb	843.62	K	Joback Method
tc	1054.75	K	Joback Method
tf	459.30	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.24	J/mol×K	843.62	Joback Method
cpg	838.64	J/mol×K	878.81	Joback Method
cpg	852.84	J/mol×K	914.00	Joback Method
cpg	865.84	J/mol×K	949.19	Joback Method
cpg	877.68	J/mol×K	984.37	Joback Method
cpg	888.36	J/mol×K	1019.56	Joback Method
cpg	897.92	J/mol×K	1054.75	Joback Method
dvisc	0.0006415	Pa×s	459.30	Joback Method
dvisc	0.0002861	Pa×s	523.35	Joback Method
dvisc	0.0001522	Pa×s	587.41	Joback Method

dvisc	0.0000916	Pa×s	651.46	Joback Method
dvisc	0.0000604	Pa×s	715.51	Joback Method
dvisc	0.0000427	Pa×s	779.57	Joback Method
dvisc	0.0000318	Pa×s	843.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405710&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume