Fumaric acid, 2-isopropoxyphenyl hept-2-yl ester

Inchi: InChI=1S/C20H28O5/c1-5-6-7-10-16(4)24-19(21)13-14-20(22)25-18-12-9-8-11-17(18)23

InchiKey: KVHCXKYCRMNSSY-BUHFOSPRSA-N

Formula: C20H28O5

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

Mol. weight [g/mol]: 348.43

Physical Properties

Property code	Value	Unit	Source
gf	-277.20	kJ/mol	Joback Method
hf	-746.23	kJ/mol	Joback Method
hfus	41.13	kJ/mol	Joback Method
hvap	82.96	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.447		Crippen Method
mcvol	285.350	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	866.94	K	Joback Method
tc	1075.65	K	Joback Method
tf	485.57	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.18	J/mol×K	866.94	Joback Method
cpg	896.58	J/mol×K	901.72	Joback Method
cpg	910.77	J/mol×K	936.51	Joback Method
cpg	923.77	J/mol×K	971.29	Joback Method
cpg	935.60	J/mol×K	1006.08	Joback Method
cpg	946.29	J/mol×K	1040.86	Joback Method
cpg	955.85	J/mol×K	1075.65	Joback Method
dvisc	0.0004923	Pa×s	485.57	Joback Method

dvisc	0.0002359	Pa×s	549.13	Joback Method
dvisc	0.0001317	Pa×s	612.69	Joback Method
dvisc	0.0000820	Pa×s	676.25	Joback Method
dvisc	0.0000554	Pa×s	739.82	Joback Method
dvisc	0.0000398	Pa×s	803.38	Joback Method
dvisc	0.0000301	Pa×s	866.94	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=U405712&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