Fumaric acid, 2-isopropoxyphenyl 2-ethylhexyl ester

Inchi: InChI=1S/C21H30O5/c1-5-7-10-17(6-2)15-24-20(22)13-14-21(23)26-19-12-9-8-11-18(19

InchiKey: RFGZZRQREVSUHI-BUHFOSPRSA-N

Formula: C21H30O5

SMILES: CCCCC(CC)COC(=O)C=CC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-268.78	kJ/mol	Joback Method
hf	-766.87	kJ/mol	Joback Method
hfus	43.72	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.695		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2437.00		NIST Webbook
rinpol	2437.00		NIST Webbook
tb	889.82	K	Joback Method
tc	1099.16	K	Joback Method
tf	496.84	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.39	J/mol×K	889.82	Joback Method
cpg	1005.77	J/mol×K	1064.27	Joback Method
cpg	995.10	J/mol×K	1029.38	Joback Method
cpg	983.25	J/mol×K	994.49	Joback Method
cpg	970.20	J/mol×K	959.60	Joback Method
cpg	955.92	J/mol×K	924.71	Joback Method
cpg	1015.29	J/mol×K	1099.16	Joback Method
dvisc	0.0000260	Pa×s	889.82	Joback Method

dvisc	0.0000345	Pa×s	824.32	Joback Method
dvisc	0.0000482	Pa×s	758.83	Joback Method
dvisc	0.0000716	Pa×s	693.33	Joback Method
dvisc	0.0001155	Pa×s	627.83	Joback Method
dvisc	0.0002084	Pa×s	562.34	Joback Method
dvisc	0.0004392	Pa×s	496.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405713&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume