Fumaric acid, 2,6-dimethoxyphenyl 2-ethylhexyl ester

Inchi: InChI=1S/C20H28O6/c1-5-7-9-15(6-2)14-25-18(21)12-13-19(22)26-20-16(23-3)10-8-11-1

InchiKey: SVCXTDDDLHQROL-OUKQBFOZSA-N

Formula: C20H28O6

SMILES: CCCCC(CC)COC(=O)C=CC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 364.43

Physical Properties

Property code	Value	Unit	Source
gf	-389.39	kJ/mol	Joback Method
hf	-884.64	kJ/mol	Joback Method
hfus	45.45	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.925		Crippen Method
mcvol	291.220	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	894.78	K	Joback Method
tc	1103.83	K	Joback Method
tf	535.32	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.39	J/mol×K	894.78	Joback Method
cpg	968.48	J/mol×K	1068.99	Joback Method
cpg	959.04	J/mol×K	1034.15	Joback Method
cpg	948.31	J/mol×K	999.31	Joback Method
cpg	936.29	J/mol×K	964.46	Joback Method
cpg	922.99	J/mol×K	929.62	Joback Method
cpg	976.64	J/mol×K	1103.83	Joback Method
dvisc	0.0000249	Pa×s	894.78	Joback Method

dvisc	0.0000320	Pa×s	834.87	Joback Method
dvisc	0.0000427	Pa×s	774.96	Joback Method
dvisc	0.0000599	Pa×s	715.05	Joback Method
dvisc	0.0000892	Pa×s	655.14	Joback Method
dvisc	0.0001441	Pa×s	595.23	Joback Method
dvisc	0.0002590	Pa×s	535.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405756&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