Fumaric acid, 2-methoxyphenyl 2-ethylhexyl ester

Inchi: InChI=1S/C19H26O5/c1-4-6-9-15(5-2)14-23-18(20)12-13-19(21)24-17-11-8-7-10-16(17)2

InchiKey: VPEKGMQVBCKKKH-OUKQBFOZSA-N

Formula: C19H26O5

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

Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-283.18	kJ/mol	Joback Method
hf	-720.31	kJ/mol	Joback Method
hfus	42.06	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.916		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	2397.00		NIST Webbook
tb	844.50	K	Joback Method
tc	1051.13	K	Joback Method
tf	489.30	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.17	J/mol×K	844.50	Joback Method
cpg	886.52	J/mol×K	1016.69	Joback Method
cpg	875.85	J/mol×K	982.25	Joback Method
cpg	864.10	J/mol×K	947.82	Joback Method
cpg	851.25	J/mol×K	913.38	Joback Method
cpg	837.28	J/mol×K	878.94	Joback Method
cpg	896.14	J/mol×K	1051.13	Joback Method
dvisc	0.0000378	Pa×s	844.50	Joback Method
dvisc	0.0000493	Pa×s	785.30	Joback Method

dvisc	0.0000669	Pa×s	726.10	Joback Method
dvisc	0.0000960	Pa×s	666.90	Joback Method
dvisc	0.0001479	Pa×s	607.70	Joback Method
dvisc	0.0002499	Pa×s	548.50	Joback Method
dvisc	0.0004795	Pa×s	489.30	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U405934&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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