Fumaric acid, 2,6-dimethoxyphenyl cyclohexylmethyl ester

Inchi: InChI=1S/C19H24O6/c1-22-15-9-6-10-16(23-2)19(15)25-18(21)12-11-17(20)24-13-14-7-

InchiKey: VOTLTLOAGBLLGE-VAWYXSNFSA-N

Formula: C19H24O6

SMILES: COc1cccc(OC)c1OC(=O)C=CC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 348.39

Physical Properties

Property code	Value	Unit	Source
gf	-370.92	kJ/mol	Joback Method
hf	-804.40	kJ/mol	Joback Method
hfus	38.22	kJ/mol	Joback Method
hvap	85.01	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.289		Crippen Method
mcvol	266.270	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
rinpol	2679.00		NIST Webbook
tb	891.89	K	Joback Method
tc	1117.49	K	Joback Method
tf	546.43	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.09	J/mol×K	891.89	Joback Method
cpg	857.93	J/mol×K	929.49	Joback Method
cpg	871.18	J/mol×K	967.09	Joback Method
cpg	882.85	J/mol×K	1004.69	Joback Method
cpg	892.94	J/mol×K	1042.29	Joback Method
cpg	901.45	J/mol×K	1079.89	Joback Method
cpg	908.38	J/mol×K	1117.49	Joback Method
dvisc	0.0002951	Pa×s	546.43	Joback Method
dvisc	0.0001715	Pa×s	604.01	Joback Method

dvisc	0.0001095	Pa×s	661.58	Joback Method
dvisc	0.0000752	Pa×s	719.16	Joback Method
dvisc	0.0000545	Pa×s	776.74	Joback Method
dvisc	0.0000414	Pa×s	834.31	Joback Method
dvisc	0.0000325	Pa×s	891.89	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=U405757&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