Fumaric acid, decyl 3,4-dimethoxyphenyl ester

Inchi: InChI=1S/C22H32O6/c1-4-5-6-7-8-9-10-11-16-27-21(23)14-15-22(24)28-18-12-13-19(25
InchiKey: QDBMQXJLGLUEKA-CCEZHUSRSA-N
Formula: C22H32O6
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)Oc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 392.49

Physical Properties

Property code	Value	Unit	Source
gf	-370.11	kJ/mol	Joback Method
hf	-920.64	kJ/mol	Joback Method
hfus	54.15	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.849		Crippen Method
mcvol	319.400	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	2998.00		NIST Webbook
tb	940.98	K	Joback Method
tc	1153.62	K	Joback Method
tf	572.86	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.29	J/mol×K	940.98	Joback Method
cpg	1042.11	J/mol×K	976.42	Joback Method
cpg	1055.50	J/mol×K	1011.86	Joback Method
cpg	1067.49	J/mol×K	1047.30	Joback Method
cpg	1078.07	J/mol×K	1082.74	Joback Method
cpg	1087.26	J/mol×K	1118.18	Joback Method
cpg	1095.07	J/mol×K	1153.62	Joback Method
dvisc	0.0001902	Pa×s	572.86	Joback Method
dvisc	0.0001095	Pa×s	634.21	Joback Method

dvisc	0.0000695	Pa×s	695.57	Joback Method
dvisc	0.0000475	Pa×s	756.92	Joback Method
dvisc	0.0000343	Pa×s	818.27	Joback Method
dvisc	0.0000260	Pa×s	879.63	Joback Method
dvisc	0.0000204	Pa×s	940.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348173&Units=SI

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

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