Fumaric acid, 2,6-dimethoxyphenyl dec-2-yl ester

Inchi: InChI=1S/C22H32O6/c1-5-6-7-8-9-10-12-17(2)27-20(23)15-16-21(24)28-22-18(25-3)13-1

InchiKey: HKXIDTVOLUTFCW-FOCLMDBBSA-N

Formula: C22H32O6

SMILES: CCCCCCCCC(C)OC(=O)C=CC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 392.49

Physical Properties

Property code	Value	Unit	Source
gf	-372.55	kJ/mol	Joback Method
hf	-925.92	kJ/mol	Joback Method
hfus	50.63	kJ/mol	Joback Method
hvap	90.87	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.848		Crippen Method
mcvol	319.400	ml/mol	McGowan Method
pc	1180.09	kPa	Joback Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook
tb	940.54	K	Joback Method
tc	1153.85	K	Joback Method
tf	557.86	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.74	J/mol×K	940.54	Joback Method
cpg	1042.56	J/mol×K	976.09	Joback Method
cpg	1055.94	J/mol×K	1011.64	Joback Method
cpg	1067.89	J/mol×K	1047.19	Joback Method
cpg	1078.41	J/mol×K	1082.75	Joback Method
cpg	1087.53	J/mol×K	1118.30	Joback Method
cpg	1095.24	J/mol×K	1153.85	Joback Method
dvisc	0.0002075	Pa×s	557.86	Joback Method

dvisc	0.0001129	Pa×s	621.64	Joback Method
dvisc	0.0000688	Pa×s	685.42	Joback Method
dvisc	0.0000456	Pa×s	749.20	Joback Method
dvisc	0.0000323	Pa×s	812.98	Joback Method
dvisc	0.0000240	Pa×s	876.76	Joback Method
dvisc	0.0000186	Pa×s	940.54	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=U405760&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

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