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

Inchi: InChI=1S/C19H26O6/c1-5-6-7-9-14(2)24-17(20)12-13-18(21)25-19-15(22-3)10-8-11-16(1

InchiKey: XUKXZSKZBQHYNZ-OUKQBFOZSA-N

Formula: C19H26O6

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

Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
gf	-397.81	kJ/mol	Joback Method
hf	-864.00	kJ/mol	Joback Method
hfus	42.86	kJ/mol	Joback Method
hvap	84.19	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.677		Crippen Method
mcvol	277.130	ml/mol	McGowan Method
pc	1453.46	kPa	Joback Method
rinpol	2475.00		NIST Webbook
tb	871.90	K	Joback Method
tc	1080.05	K	Joback Method
tf	524.05	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.64	J/mol×K	871.90	Joback Method
cpg	909.67	J/mol×K	1045.35	Joback Method
cpg	900.12	J/mol×K	1010.66	Joback Method
cpg	889.35	J/mol×K	975.97	Joback Method
cpg	877.35	J/mol×K	941.28	Joback Method
cpg	864.11	J/mol×K	906.59	Joback Method
cpg	917.97	J/mol×K	1080.05	Joback Method
dvisc	0.0000288	Pa×s	871.90	Joback Method
dvisc	0.0000368	Pa×s	813.92	Joback Method

dvisc	0.0000490	Pa×s	755.95	Joback Method
dvisc	0.0000683	Pa×s	697.97	Joback Method
dvisc	0.0001011	Pa×s	640.00	Joback Method
dvisc	0.0001620	Pa×s	582.02	Joback Method
dvisc	0.0002878	Pa×s	524.05	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=U405754&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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