Fumaric acid, 2,6-dimethoxyphenyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C18H20O6/c1-5-8-13(6-2)23-16(19)11-12-17(20)24-18-14(21-3)9-7-10-15(18)2

InchiKey: QFGYTLQFUVWRST-VAWYXSNFSA-N

Formula: C18H20O6

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

Mol. weight [g/mol]: 332.35

Physical Properties

Property code	Value	Unit	Source
gf	-203.43	kJ/mol	Joback Method
hf	-571.06	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	2.510		Crippen Method
mcvol	254.440	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	858.02	K	Joback Method
tc	1080.34	K	Joback Method
tf	618.88	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.02	J/mol×K	858.02	Joback Method
cpg	752.59	J/mol×K	895.07	Joback Method
cpg	764.92	J/mol×K	932.13	Joback Method
cpg	775.99	J/mol×K	969.18	Joback Method
cpg	785.79	J/mol×K	1006.23	Joback Method
cpg	794.32	J/mol×K	1043.28	Joback Method
cpg	801.56	J/mol×K	1080.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405753&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
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