Fumaric acid, 2,6-dimethoxyphenyl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C25H34O6/c1-4-5-6-7-8-9-10-11-12-13-14-20-30-23(26)18-19-24(27)31-25-21

InchiKey: APPSVOZDNNVMKI-VHEBQXMUSA-N

Formula: C25H34O6

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

Mol. weight [g/mol]: 430.53

Physical Properties

Property code	Value	Unit	Source
gf	-142.05	kJ/mol	Joback Method
hf	-710.26	kJ/mol	Joback Method
hfus	65.04	kJ/mol	Joback Method
hvap	100.09	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.243		Crippen Method
mcvol	353.070	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
rinpol	3128.00		NIST Webbook
rinpol	3128.00		NIST Webbook
tb	1018.62	K	Joback Method
tc	1247.25	K	Joback Method
tf	712.77	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.23	J/mol×K	1018.62	Joback Method
cpg	1166.11	J/mol×K	1056.73	Joback Method
cpg	1178.30	J/mol×K	1094.83	Joback Method
cpg	1188.82	J/mol×K	1132.94	Joback Method
cpg	1197.69	J/mol×K	1171.04	Joback Method
cpg	1204.91	J/mol×K	1209.15	Joback Method
cpg	1210.52	J/mol×K	1247.25	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=U405763&Units=SI

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