Fumaric acid, 4-methoxyphenyl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C24H32O5/c1-3-4-5-6-7-8-9-10-11-12-13-20-28-23(25)18-19-24(26)29-22-16-1

InchiKey: VWTWKABZFALWOL-VHEBQXMUSA-N

Formula: C24H32O5

SMILES: CCCCCCCCCCC#CCOC(=O)C=CC(=O)Oc1ccc(OC)cc1

Mol. weight [g/mol]: 400.51

Physical Properties

Property code	Value	Unit	Source
gf	-35.84	kJ/mol	Joback Method
hf	-545.93	kJ/mol	Joback Method
hfus	61.65	kJ/mol	Joback Method
hvap	94.79	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.234		Crippen Method
mcvol	333.110	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	3063.00		NIST Webbook
rinpol	3063.00		NIST Webbook
tb	968.34	K	Joback Method
tc	1188.83	K	Joback Method
tf	666.75	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.84	J/mol×K	968.34	Joback Method
cpg	1079.76	J/mol×K	1005.09	Joback Method
cpg	1093.31	J/mol×K	1041.84	Joback Method
cpg	1105.51	J/mol×K	1078.59	Joback Method
cpg	1116.42	J/mol×K	1115.33	Joback Method
cpg	1126.05	J/mol×K	1152.08	Joback Method
cpg	1134.46	J/mol×K	1188.83	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=U405785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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