Fumaric acid, 3-phenylpropyl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C26H36O4/c1-2-3-4-5-6-7-8-9-10-11-15-22-29-25(27)20-21-26(28)30-23-16-19

InchiKey: UVRMUMLPAFYPES-QZQOTICOSA-N

Formula: C26H36O4

SMILES: CCCCCCCCCCC#CCOC(=O)C=CC(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 412.56

Physical Properties

Property code	Value	Unit	Source
gf	95.63	kJ/mol	Joback Method
hf	-443.52	kJ/mol	Joback Method
hfus	66.03	kJ/mol	Joback Method
hvap	96.17	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.796		Crippen Method
mcvol	355.420	ml/mol	McGowan Method
pc	1054.83	kPa	Joback Method
rinpol	3098.00		NIST Webbook
rinpol	3098.00		NIST Webbook
tb	986.70	K	Joback Method
tc	1209.16	K	Joback Method
tf	654.54	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1159.54	J/mol×K	986.70	Joback Method
cpg	1175.74	J/mol×K	1023.78	Joback Method
cpg	1190.63	J/mol×K	1060.85	Joback Method
cpg	1204.31	J/mol×K	1097.93	Joback Method
cpg	1216.82	J/mol×K	1135.01	Joback Method
cpg	1228.25	J/mol×K	1172.08	Joback Method
cpg	1238.65	J/mol×K	1209.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405673&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

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