(E)-1-(3,4-Dimethoxyphenyl)tetradec-4-en-3-one

Inchi: InChI=1S/C22H34O3/c1-4-5-6-7-8-9-10-11-12-13-20(23)16-14-19-15-17-21(24-2)22(18-1
InchiKey: KKRNHCNPKJGKDR-OUKQBFOZSA-N
Formula: C22H34O3
SMILES: CCCCCCCCCC=CC(=O)CCc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 346.50

Physical Properties

Property code	Value	Unit	Source
gf	-31.19	kJ/mol	Joback Method
hf	-543.62	kJ/mol	Joback Method
hfus	50.18	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.902		Crippen Method
mcvol	306.090	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	2739.80		NIST Webbook
rinpol	2739.80		NIST Webbook
tb	842.27	K	Joback Method
tc	1040.66	K	Joback Method
tf	478.47	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.27	J/mol×K	842.27	Joback Method
cpg	967.99	J/mol×K	875.34	Joback Method
cpg	984.61	J/mol×K	908.40	Joback Method
cpg	1000.16	J/mol×K	941.47	Joback Method
cpg	1014.67	J/mol×K	974.53	Joback Method
cpg	1028.18	J/mol×K	1007.60	Joback Method
cpg	1040.71	J/mol×K	1040.66	Joback Method
dvisc	0.0004675	Pa×s	478.47	Joback Method

dvisc	0.0002433	Pa×s	539.10	Joback Method
dvisc	0.0001444	Pa×s	599.74	Joback Method
dvisc	0.0000944	Pa×s	660.37	Joback Method
dvisc	0.0000662	Pa×s	721.00	Joback Method
dvisc	0.0000491	Pa×s	781.64	Joback Method
dvisc	0.0000380	Pa×s	842.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412871&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
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