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

Inchi: InChI=1S/C20H30O3/c1-4-5-6-7-8-9-10-11-18(21)14-12-17-13-15-19(22-2)20(16-17)23-3
InchiKey: ZNOLGYFCFIVHQI-ZHACJKMWSA-N
Formula: C20H30O3
SMILES: CCCCCCCC=CC(=O)CCc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 318.45
CAS: 863780-79-4

Physical Properties

Property code	Value	Unit	Source
gf	-48.03	kJ/mol	Joback Method
hf	-502.34	kJ/mol	Joback Method
hfus	45.00	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.122		Crippen Method
mcvol	277.910	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinpol	2533.50		NIST Webbook
tb	796.51	K	Joback Method
tc	993.89	K	Joback Method
tf	455.93	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.32	J/mol×K	796.51	Joback Method
cpg	848.56	J/mol×K	829.41	Joback Method
cpg	864.76	J/mol×K	862.30	Joback Method
cpg	879.96	J/mol×K	895.20	Joback Method
cpg	894.17	J/mol×K	928.10	Joback Method
cpg	907.44	J/mol×K	960.99	Joback Method
cpg	919.78	J/mol×K	993.89	Joback Method
dvisc	0.0005641	Pa×s	455.93	Joback Method

dvisc	0.0003007	Pa×s	512.69	Joback Method
dvisc	0.0001817	Pa×s	569.46	Joback Method
dvisc	0.0001203	Pa×s	626.22	Joback Method
dvisc	0.0000853	Pa×s	682.98	Joback Method
dvisc	0.0000637	Pa×s	739.75	Joback Method
dvisc	0.0000497	Pa×s	796.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C863780794&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