

(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:	ZNOLGYFCFIVHQB-ZHACJKMWSA-N
Formula:	C20H30O3
SMILES:	CCCCCCC=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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003007	Paxs	512.69	Joback Method
dvisc	0.0001817	Paxs	569.46	Joback Method
dvisc	0.0001203	Paxs	626.22	Joback Method
dvisc	0.0000853	Paxs	682.98	Joback Method
dvisc	0.0000637	Paxs	739.75	Joback Method
dvisc	0.0000497	Paxs	796.51	Joback Method

Sources

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=C863780794&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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