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

Inchi: InChI=1S/C18H26O3/c1-4-5-6-7-8-9-16(19)12-10-15-11-13-17(20-2)18(14-15)21-3/h8-9,
InchiKey: NBXXCGNHVWDCHB-CMDGGOBGSA-N
Formula: C18H26O3
SMILES: CCCCCC=CC(=O)CCc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 290.40
CAS: 79067-86-0

Physical Properties

Property code	Value	Unit	Source
gf	-64.87	kJ/mol	Joback Method
hf	-461.06	kJ/mol	Joback Method
hfus	39.82	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.342		Crippen Method
mcvol	249.730	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	2328.80		NIST Webbook
rinpol	2328.80		NIST Webbook
tb	750.75	K	Joback Method
tc	949.60	K	Joback Method
tf	433.39	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.00	J/mol×K	750.75	Joback Method
cpg	732.70	J/mol×K	783.89	Joback Method
cpg	748.43	J/mol×K	817.03	Joback Method
cpg	763.21	J/mol×K	850.18	Joback Method
cpg	777.06	J/mol×K	883.32	Joback Method
cpg	790.01	J/mol×K	916.46	Joback Method
cpg	802.07	J/mol×K	949.60	Joback Method

dvisc	0.0006665	Pa×s	433.39	Joback Method
dvisc	0.0003647	Pa×s	486.28	Joback Method
dvisc	0.0002246	Pa×s	539.18	Joback Method
dvisc	0.0001508	Pa×s	592.07	Joback Method
dvisc	0.0001081	Pa×s	644.96	Joback Method
dvisc	0.0000815	Pa×s	697.86	Joback Method
dvisc	0.0000640	Pa×s	750.75	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79067860&Units=SI

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