(E)-1-(4-Hydroxy-3-methoxyphenyl)dec-3-en-5-one

Inchi: InChI=1S/C17H24O3/c1-3-4-5-9-15(18)10-7-6-8-14-11-12-16(19)17(13-14)20-2/h7,10-13
InchiKey: CERFNDVNLCZPSE-JXMROGBWSA-N
Formula: C17H24O3
SMILES: CCCCCC(=O)C=CCCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 276.37
CAS: 863913-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-113.28	kJ/mol	Joback Method
hf	-474.04	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	78.50	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.039		Crippen Method
mcvol	235.640	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2231.70		NIST Webbook
rinpol	2231.70		NIST Webbook
tb	781.09	K	Joback Method
tc	990.84	K	Joback Method
tf	499.09	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.80	J/mol×K	781.09	Joback Method
cpg	705.04	J/mol×K	816.05	Joback Method
cpg	719.49	J/mol×K	851.01	Joback Method
cpg	733.24	J/mol×K	885.96	Joback Method
cpg	746.37	J/mol×K	920.92	Joback Method
cpg	758.95	J/mol×K	955.88	Joback Method
cpg	771.06	J/mol×K	990.84	Joback Method

dvisc	0.0001845	Pa×s	499.09	Joback Method
dvisc	0.0000813	Pa×s	546.09	Joback Method
dvisc	0.0000408	Pa×s	593.09	Joback Method
dvisc	0.0000227	Pa×s	640.09	Joback Method
dvisc	0.0000136	Pa×s	687.09	Joback Method
dvisc	0.0000088	Pa×s	734.09	Joback Method
dvisc	0.0000059	Pa×s	781.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C863913659&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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