1-(4-Hydroxy-3-methoxyphenyl)dodec-4-en-3-one

Other names: [8]-Shogaol
4-Dodecen-3-one, 1-(4-hydroxy-3-methoxyphenyl)
Inchi: InChI=1S/C19H28O3/c1-3-4-5-6-7-8-9-10-17(20)13-11-16-12-14-18(21)19(15-16)22-2/h9
InchiKey: LGZSMXJRMTYABD-MDZDMXLPSA-N
Formula: C19H28O3
SMILES: CCCCCCCC=CC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 304.42
CAS: 36700-45-5

Physical Properties

Property code	Value	Unit	Source
gf	-96.44	kJ/mol	Joback Method
hf	-515.32	kJ/mol	Joback Method
hfus	47.39	kJ/mol	Joback Method
hvap	82.95	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.819		Crippen Method
mcvol	263.820	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2275.00		NIST Webbook
tb	826.85	K	Joback Method
tc	1034.02	K	Joback Method
tf	521.63	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.94	J/mol×K	826.85	Joback Method
cpg	877.15	J/mol×K	999.49	Joback Method
cpg	863.74	J/mol×K	964.96	Joback Method
cpg	849.79	J/mol×K	930.44	Joback Method
cpg	835.23	J/mol×K	895.91	Joback Method
cpg	819.97	J/mol×K	861.38	Joback Method

cpg	890.12	J/mol×K	1034.02	Joback Method
dvisc	0.0000039	Pa×s	826.85	Joback Method
dvisc	0.0000058	Pa×s	775.98	Joback Method
dvisc	0.0000091	Pa×s	725.11	Joback Method
dvisc	0.0000152	Pa×s	674.24	Joback Method
dvisc	0.0000277	Pa×s	623.37	Joback Method
dvisc	0.0000560	Pa×s	572.50	Joback Method
dvisc	0.0001298	Pa×s	521.63	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36700455&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

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