

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

Other names:	4-Decen-3-one, 1-(4-hydroxy-3-methoxyphenyl)- Shogaol (6)-Shogaol
Inchi:	InChI=1S/C17H24O3/c1-3-4-5-6-7-8-15(18)11-9-14-10-12-16(19)17(13-14)20-2/h7-8,10,
InchiKey:	OQWKEEOHDMUXEO-BQYQJAHWSA-N
Formula:	C17H24O3
SMILES:	CCCCC=CC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]:	276.37
CAS:	555-66-8

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	2294.00		NIST Webbook
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook
rinpol	2294.00		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/molxK	781.09	Joback Method
cpg	758.95	J/molxK	955.88	Joback Method

cpg	746.37	J/molxK	920.92	Joback Method
cpg	733.24	J/molxK	885.96	Joback Method
cpg	719.49	J/molxK	851.01	Joback Method
cpg	705.04	J/molxK	816.05	Joback Method
cpg	771.06	J/molxK	990.84	Joback Method
dvisc	0.0000059	Paxs	781.09	Joback Method
dvisc	0.0000088	Paxs	734.09	Joback Method
dvisc	0.0000136	Paxs	687.09	Joback Method
dvisc	0.0000227	Paxs	640.09	Joback Method
dvisc	0.0000408	Paxs	593.09	Joback Method
dvisc	0.0000813	Paxs	546.09	Joback Method
dvisc	0.0001845	Paxs	499.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C555668&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

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