

6-(3-Hydroxy-4-methylphenyl)-2-methylhept-2-en-

Other names:	Turmeronol A 2-Hepten-4-one, 6-(3-hydroxy-4-methylphenyl)-2-methyl- 2-Hepten-4-one, 2-methyl-6-(3-hydroxy-4-methylphenyl)
Inchi:	InChI=1S/C15H20O2/c1-10(2)7-14(16)8-12(4)13-6-5-11(3)15(17)9-13/h5-7,9,12,17H,8H2
InchiKey:	OSIFVLKZUWRNBN-UHFFFAOYSA-N
Formula:	C15H20O2
SMILES:	CC(C)=CC(=O)CC(C)c1ccc(C)c(O)c1
Mol. weight [g/mol]:	232.32
CAS:	139085-16-8

Physical Properties

Property code	Value	Unit	Source
gf	-36.11	kJ/mol	Joback Method
hf	-315.61	kJ/mol	Joback Method
hfus	31.01	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.730		Crippen Method
mcvol	201.590	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinsol	1733.00		NIST Webbook
rinsol	1733.00		NIST Webbook
tb	712.35	K	Joback Method
tc	936.34	K	Joback Method
tf	425.36	K	Joback Method
vc	0.715	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.78	J/mol×K	712.35	Joback Method
cpg	568.91	J/mol×K	749.68	Joback Method
cpg	583.16	J/mol×K	787.01	Joback Method
cpg	596.63	J/mol×K	824.35	Joback Method

cpg	609.43	J/mol×K	861.68	Joback Method
cpg	621.66	J/mol×K	899.01	Joback Method
cpg	633.43	J/mol×K	936.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C139085168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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