

trans-5-Hydroxy-p-menth-1(6)-en-2-one

Inchi:	InChI=1S/C10H16O2/c1-6(2)8-5-9(11)7(3)4-10(8)12/h4,6,8,10,12H,5H2,1-3H3/t8-,10+/m
InchiKey:	ZFUJCNJIGDBFEP-SCZZXKLOSA-N
Formula:	C10H16O2
SMILES:	CC1=CC(O)C(C(C)C)CC1=O
Mol. weight [g/mol]:	168.23

Physical Properties

Property code	Value	Unit	Source
gf	-191.46	kJ/mol	Joback Method
hf	-464.65	kJ/mol	Joback Method
hfus	15.47	kJ/mol	Joback Method
hvap	59.47	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.539		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinsol	1410.00		NIST Webbook
rinsol	1410.00		NIST Webbook
tb	606.78	K	Joback Method
tc	812.40	K	Joback Method
tf	332.92	K	Joback Method
vc	0.533	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.06	J/mol×K	606.78	Joback Method
cpg	398.33	J/mol×K	641.05	Joback Method
cpg	412.83	J/mol×K	675.32	Joback Method
cpg	426.57	J/mol×K	709.59	Joback Method
cpg	439.53	J/mol×K	743.86	Joback Method
cpg	451.71	J/mol×K	778.13	Joback Method
cpg	463.09	J/mol×K	812.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233919&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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