

6-Hydroxy-1,1,4,4-tetramethyl-1,2,3,4-tetrahydrona

Inchi:	InChI=1S/C14H20O/c1-13(2)7-8-14(3,4)12-9-10(15)5-6-11(12)13/h5-6,9,15H,7-8H2,1-4H
InchiKey:	UZHCJGSIRIFQTO-UHFFFAOYSA-N
Formula:	C14H20O
SMILES:	CC1(C)CCC(C)(C)c2cc(O)ccc21
Mol. weight [g/mol]:	204.31
CAS:	22824-31-3

Physical Properties

Property code	Value	Unit	Source
gf	45.12	kJ/mol	Joback Method
hf	-207.76	kJ/mol	Joback Method
hfus	15.96	kJ/mol	Joback Method
hvap	60.18	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.741		Crippen Method
mcvol	179.370	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
tb	638.82	K	Joback Method
tc	883.51	K	Joback Method
tf	456.18	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.35	J/molxK	638.82	Joback Method
cpg	506.00	J/molxK	679.60	Joback Method
cpg	522.80	J/molxK	720.38	Joback Method
cpg	539.14	J/molxK	761.17	Joback Method
cpg	555.39	J/molxK	801.95	Joback Method
cpg	571.93	J/molxK	842.73	Joback Method
cpg	589.13	J/molxK	883.51	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22824313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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