

(S,Z)-5-Hydroxy-6-methyl-2-((2S,5R)-5-methyl-5-vi

Inchi:	InChI=1S/C15H22O3/c1-6-15(5)8-7-14(18-15)11(4)13(17)9-12(16)10(2)3/h6,9,11,14,16H
InchiKey:	AYJCMTOVQWMEDB-XFXZXTDPSA-N
Formula:	C15H22O3
SMILES:	<chem>C=CC1(C)CCC(C(C)C(=O)C=C(O)C(=C)C)O1</chem>
Mol. weight [g/mol]:	250.33
CAS:	160114-70-5

Physical Properties

Property code	Value	Unit	Source
gf	-16.73	kJ/mol	Joback Method
hf	-351.14	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	74.11	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.333		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1644.70		NIST Webbook
rinpol	1644.70		NIST Webbook
tb	723.29	K	Joback Method
tc	928.14	K	Joback Method
tf	375.17	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.13	J/molxK	723.29	Joback Method
cpg	629.75	J/molxK	757.43	Joback Method
cpg	644.72	J/molxK	791.57	Joback Method
cpg	659.19	J/molxK	825.72	Joback Method
cpg	673.29	J/molxK	859.86	Joback Method
cpg	687.15	J/molxK	894.00	Joback Method
cpg	700.90	J/molxK	928.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C160114705&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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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