Silphiperfol-5-en-3-ol C

Inchi: InChI=1S/C15H24O/c1-9-5-6-15-11(3)10(2)8-14(15,4)13(16)7-12(9)15/h8-9,11-13,16H,5
InchiKey: KACKPLUHPMMFBK-UXKQUHDHSA-N
Formula: C15H24O
SMILES: CC1=CC2(C)C(O)CC3C(C)CCC32C1C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	82.87	kJ/mol	Joback Method
hf	-283.31	kJ/mol	Joback Method
hfus	20.35	kJ/mol	Joback Method
hvap	63.47	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	654.15	K	Joback Method
tc	862.88	K	Joback Method
tf	414.77	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.39	J/mol×K	654.15	Joback Method
cpg	595.29	J/mol×K	688.94	Joback Method
cpg	613.37	J/mol×K	723.73	Joback Method
cpg	630.87	J/mol×K	758.52	Joback Method
cpg	648.01	J/mol×K	793.31	Joback Method
cpg	665.02	J/mol×K	828.10	Joback Method
cpg	682.13	J/mol×K	862.88	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=R226832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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