Silphiperfol-6-en-5-one

Inchi: InChI=1S/C15H22O/c1-9-5-8-15-11(3)10(2)13(16)14(15,4)7-6-12(9)15/h9,12H,5-8H2,1-4
InchiKey: WRSMTJOLBOXBOD-UXLHTXSSSA-N
Formula: C15H22O
SMILES: CC1=C(C)C23CCC(C)C2CCC3(C)C1=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
hfus	13.24	kJ/mol	Joback Method
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
rinpol	1623.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1607.00		NIST Webbook
ripol	2125.00		NIST Webbook
ripol	2163.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.11	J/mol×K	644.11	Joback Method
cpg	562.10	J/mol×K	684.01	Joback Method
cpg	582.11	J/mol×K	723.92	Joback Method
cpg	601.45	J/mol×K	763.82	Joback Method
cpg	620.44	J/mol×K	803.73	Joback Method
cpg	639.37	J/mol×K	843.63	Joback Method
cpg	658.57	J/mol×K	883.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R499515&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices