

Silphiperfol-6-ene

Other names:	(-)-Silphiperfol-6-ene
Inchi:	InChI=1S/C15H24/c1-10-5-8-15-12(3)11(2)9-14(15,4)7-6-13(10)15/h10,13H,5-9H2,1-4H3
InchiKey:	VIXZYZFZHINXMQ-KQLPNOJUSA-N
Formula:	C15H24
SMILES:	CC1=C(C)C23CCC(C)C2CCC3(C)C1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
hfus	13.73	kJ/mol	Joback Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
rinpol	1376.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1365.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1496.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.46	J/mol×K	576.29	Joback Method

cpg	525.54	J/mol×K	614.06	Joback Method
cpg	546.15	J/mol×K	651.82	Joback Method
cpg	565.60	J/mol×K	689.59	Joback Method
cpg	584.18	J/mol×K	727.36	Joback Method
cpg	602.19	J/mol×K	765.12	Joback Method
cpg	619.93	J/mol×K	802.89	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R226298&Units=SI
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
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

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