

Silhiperfol-5-en-3-one A

Inchi:	InChI=1S/C15H22O/c1-9-5-6-15-11(3)10(2)8-14(15,4)13(16)7-12(9)15/h8-9,11-12H,5-7H
InchiKey:	WTORUARCGCVBSQ-GJDKHMSTSA-N
Formula:	C15H22O
SMILES:	CC1=CC2(C)C(=O)CC3C(C)CCC32C1C
Mol. weight [g/mol]:	218.33
CAS:	138752-21-3

Physical Properties

Property code	Value	Unit	Source
gf	104.81	kJ/mol	Joback Method
hf	-248.44	kJ/mol	Joback Method
hfus	14.70	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	634.46	K	Joback Method
tc	873.09	K	Joback Method
tf	426.41	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.90	J/mol×K	634.46	Joback Method
cpg	564.64	J/mol×K	674.23	Joback Method
cpg	585.28	J/mol×K	714.00	Joback Method
cpg	605.11	J/mol×K	753.77	Joback Method
cpg	624.46	J/mol×K	793.54	Joback Method
cpg	643.61	J/mol×K	833.32	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=C138752213&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

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