

Spirafolide

Inchi:	InChI=1S/C15H18O3/c1-9-8-17-7-6-15(3)5-4-11-10(2)14(16)18-13(11)12(9)15/h6-8,11-1
InchiKey:	CHJVABAWMKQXSI-UHFFFAOYSA-N
Formula:	C15H18O3
SMILES:	<chem>C=C1C(=O)OC2C1CCC1(C)C=COC=C(C)C21</chem>
Mol. weight [g/mol]:	246.30
CAS:	130838-06-1

Physical Properties

Property code	Value	Unit	Source
gf	-7.49	kJ/mol	Joback Method
hf	-383.80	kJ/mol	Joback Method
hfus	29.65	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.948		Crippen Method
mcvol	190.040	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	1993.90		NIST Webbook
tb	703.92	K	Joback Method
tc	954.02	K	Joback Method
tf	463.77	K	Joback Method
vc	0.709	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.20	J/mol×K	703.92	Joback Method
cpg	591.29	J/mol×K	745.60	Joback Method
cpg	610.24	J/mol×K	787.29	Joback Method
cpg	628.24	J/mol×K	828.97	Joback Method
cpg	645.46	J/mol×K	870.65	Joback Method
cpg	662.09	J/mol×K	912.34	Joback Method
cpg	678.30	J/mol×K	954.02	Joback Method

Sources

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=C130838061&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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