

Drimenin

Inchi:	InChI=1S/C15H22O2/c1-14(2)7-4-8-15(3)11(14)6-5-10-9-17-13(16)12(10)15/h5,11-12H,4
InchiKey:	BQNSBENKJCLJGN-BQELKBSMSA-N
Formula:	C15H22O2
SMILES:	CC1(C)CCCC2(C)C3C(=O)OCC3=CCC12
Mol. weight [g/mol]:	234.33

Physical Properties

Property code	Value	Unit	Source
gf	2.20	kJ/mol	Joback Method
hf	-372.42	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	56.51	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.322		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinqol	1929.00		NIST Webbook
tb	674.62	K	Joback Method
tc	925.69	K	Joback Method
tf	450.18	K	Joback Method
vc	0.724	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.85	J/mol×K	674.62	Joback Method
cpg	602.24	J/mol×K	716.46	Joback Method
cpg	623.65	J/mol×K	758.31	Joback Method
cpg	644.41	J/mol×K	800.15	Joback Method
cpg	664.86	J/mol×K	842.00	Joback Method
cpg	685.33	J/mol×K	883.84	Joback Method
cpg	706.18	J/mol×K	925.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R517752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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