

Corymbolone

Other names:	(4S,4aR,6R,8aR)-4a-Hydroxy-4,8a-dimethyl-6-(prop-1-en-2-yl)octahydronaphthalen-1(2H)
Inchi:	InChI=1S/C15H24O2/c1-10(2)12-7-8-14(4)13(16)6-5-11(3)15(14,17)9-12/h11-12,17H,1,5
InchiKey:	BMGSSZITOGSORO-UHFFFAOYSA-N
Formula:	C15H24O2
SMILES:	<chem>C=C(C)C1CCC2(C)C(=O)CCC(C)C2(O)C1</chem>
Mol. weight [g/mol]:	236.35
CAS:	97094-19-4

Physical Properties

Property code	Value	Unit	Source
gf	-58.00	kJ/mol	Joback Method
hf	-416.46	kJ/mol	Joback Method
hfus	13.03	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.099		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1898.70		NIST Webbook
tb	720.86	K	Joback Method
tc	944.74	K	Joback Method
tf	433.25	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.25	J/molxK	720.86	Joback Method
cpg	651.36	J/molxK	758.17	Joback Method
cpg	670.87	J/molxK	795.49	Joback Method
cpg	689.99	J/molxK	832.80	Joback Method
cpg	708.95	J/molxK	870.11	Joback Method
cpg	727.97	J/molxK	907.42	Joback Method
cpg	747.25	J/molxK	944.74	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=C97094194&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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