

(E)-15,16-Dinorlabda-8(17),12-dien-14-al

Inchi:	InChI=1S/C18H28O/c1-14-9-10-16-17(2,3)11-7-12-18(16,4)15(14)8-5-6-13-19/h5-6,13,15
InchiKey:	UMOQQBYJZPZYPC-AATRIKPKSA-N
Formula:	C18H28O
SMILES:	<chem>C=C1CCC2C(C)(C)CCCC2(C)C1CC=CC=O</chem>
Mol. weight [g/mol]:	260.41
CAS:	167817-63-2

Physical Properties

Property code	Value	Unit	Source
gf	181.16	kJ/mol	Joback Method
hf	-188.21	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	60.09	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.930		Crippen Method
mcvol	235.730	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	1967.40		NIST Webbook
rinpol	1948.00		NIST Webbook
rinpol	1948.00		NIST Webbook
rinpol	1967.40		NIST Webbook
tb	684.92	K	Joback Method
tc	907.53	K	Joback Method
tf	404.34	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.60	J/molxK	684.92	Joback Method
cpg	714.07	J/molxK	722.02	Joback Method
cpg	735.62	J/molxK	759.12	Joback Method
cpg	756.51	J/molxK	796.23	Joback Method
cpg	776.99	J/molxK	833.33	Joback Method

cpg	797.31	J/mol×K	870.43	Joback Method
cpg	817.75	J/mol×K	907.53	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=C167817632&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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