Zeranol

Other names:

1H-2-Benzoxacyclotetradecin-1-one, 3,4,5,6,7,8,9,10,11,12-decahydro-7,14,16-trihydroxy-3-methyl-, [3S-(3R*,7S*)]-

1H-2-Benzoxacyclotetradecin-1-one, 3,4,5,6,7,8,9,10,11,12-decahydro-7,14,16-trihydroxy-3-methyl-, (3S,7R)-(+)-

MK-188

P 1496

Ralgro

Zearalanol

Zearanol

1H-2-Benzoxacyclotetradecin-1-one, 3,4,5,6,7,8,9,10,11,12-decahydro-7,14,16-trihydroxy-3-methyl-, (3S,7X)-

6-(6,10-Dihydroxyundecyl)-«beta»-resorcylic acid, «mu»-lactone

Frideron

Ralabol

Ralone

(3S,7X)-3,4,5,6,7,8,9,10,11,12-Decahydro-7,14,16-trihydroxy-3-methyl-1H-2-benzoxacycl

(6X,10S)-6-(6,10-Dihydroxyundecyl)-«beta»-resorcylic acid «mu»-lactone

THFES(HM)

7,14,16-Trihydroxy-3-methyl-3,4,5,6,7,8,9,10,11,12-decahydro-1H-2-benzoxacyclotetrade

1H-2-Benzoxacyclotetradecin-1-one, 3,4,5,6,7,8,9,10,11,12-decahydro-7,14,16-trihydroxy-3-methyl-, (3S,7R)-

«alpha»-Zearalanol

Zeranol (2,4-Dihydroxy-6-(6A,10-dihydroxy-trans-1-undecenylbenzoic acid) mu-lactone), TMS

Inchi: InChI=1S/C18H26O5/c1-12-6-5-9-14(19)8-4-2-3-7-13-10-15(20)11-16(21)17(13)18(22)23

InchiKey: DWTTZBARDOXEAM-UHFFFAOYSA-N

Formula: C18H26O5

SMILES: CC1CCCC(O)CCCCCc2cc(O)cc(O)c2C(=O)O1

Mol. weight [g/mol]: 322.40

CAS: 26538-44-3

Physical Properties

Property code	Value	Unit	Source
gf	-507.17	kJ/mol	Joback Method
hf	-969.32	kJ/mol	Joback Method
hfus	39.48	kJ/mol	Joback Method
hvap	111.22	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.291		Crippen Method
mcvol	254.910	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	2842.00		NIST Webbook

rinpol	2842.00		NIST Webbook
tb	1031.59	K	Joback Method
tc	1289.68	K	Joback Method
tf	692.63	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.91	J/mol×K	1031.59	Joback Method
cpg	935.34	J/mol×K	1074.61	Joback Method
cpg	947.16	J/mol×K	1117.62	Joback Method
cpg	957.45	J/mol×K	1160.64	Joback Method
cpg	966.26	J/mol×K	1203.65	Joback Method
cpg	973.70	J/mol×K	1246.67	Joback Method
cpg	979.82	J/mol×K	1289.68	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=C26538443&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