

Platambin

Inchi:	InChI=1S/C15H26O2/c1-9(2)11-7-8-15(4)12(16)6-5-10(3)13(15)14(11)17/h9,11-14,16-17
InchiKey:	WKKJGHCXVKEJNU-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	<chem>C=C1CCC(O)C2(C)CCC(C(C)C)C(O)C12</chem>
Mol. weight [g/mol]:	238.37
CAS:	58556-80-2

Physical Properties

Property code	Value	Unit	Source
gf	-103.10	kJ/mol	Joback Method
hf	-503.25	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.747		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1867.00		NIST Webbook
ripol	2686.00		NIST Webbook
tb	742.47	K	Joback Method
tc	937.28	K	Joback Method
tf	412.11	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.64	J/molxK	742.47	Joback Method
cpg	687.05	J/molxK	774.94	Joback Method
cpg	703.74	J/molxK	807.41	Joback Method
cpg	719.81	J/molxK	839.87	Joback Method
cpg	735.35	J/molxK	872.34	Joback Method
cpg	750.45	J/molxK	904.81	Joback Method
cpg	765.20	J/molxK	937.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58556802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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