

urs-12-ene-3«beta»,28-diol

Other names:	Uvaol
Inchi:	InChI=1S/C30H50O2/c1-19-10-15-30(18-31)17-16-28(6)21(25(30)20(19)2)8-9-23-27(5)1
InchiKey:	XUARCIYIVXVTAE-UHFFFAOYSA-N
Formula:	C30H50O2
SMILES:	CC1CCC2(CO)CCC3(C)C(=CCC4C5(C)CCC(O)C(C)(C)C5CCC43C)C2C1C
Mol. weight [g/mol]:	442.72
CAS:	545-46-0

Physical Properties

Property code	Value	Unit	Source
gf	93.75	kJ/mol	Joback Method
hf	-645.64	kJ/mol	Joback Method
hfus	33.38	kJ/mol	Joback Method
hvap	109.85	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.997		Crippen Method
mcvol	386.700	ml/mol	McGowan Method
pc	1081.35	kPa	Joback Method
rinpol	3692.40		NIST Webbook
rinpol	3692.40		NIST Webbook
tb	1111.07	K	Joback Method
tc	1360.43	K	Joback Method
tf	721.90	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1714.79	J/molxK	1111.07	Joback Method
cpg	1784.17	J/molxK	1152.63	Joback Method
cpg	1860.65	J/molxK	1194.19	Joback Method
cpg	1945.08	J/molxK	1235.75	Joback Method
cpg	2038.29	J/molxK	1277.31	Joback Method
cpg	2141.12	J/molxK	1318.87	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=C545460&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
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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