

Uvaol

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]:	442.73

Physical Properties

Property code	Value	Unit	Source
hfus	33.38	kJ/mol	Joback Method
logp	6.997		Crippen Method
mcvol	386.700	ml/mol	McGowan Method
rinpol	3692.40		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1714.79	J/mol×K	1111.07	Joback Method
cpg	1784.17	J/mol×K	1152.63	Joback Method
cpg	1860.65	J/mol×K	1194.19	Joback Method
cpg	1945.08	J/mol×K	1235.75	Joback Method
cpg	2038.29	J/mol×K	1277.31	Joback Method
cpg	2141.12	J/mol×K	1318.87	Joback Method
cpg	2254.43	J/mol×K	1360.43	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C545460&Units=SI>

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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