

«alpha»-Amyrin

Other names:	Urs-12-en-3-ol, (3«beta»)- Urs-12-en-3«beta»-ol «alpha»-Amyrenol «alpha»-Amyrine Viminalol «alpha»-Amirine Urs-12-en-3-ol
Inchi:	InChI=1S/C30H50O/c1-19-11-14-27(5)17-18-29(7)21(25(27)20(19)2)9-10-23-28(6)15-13
InchiKey:	FSLPMRQHCOLESF-UHFFFAOYSA-N
Formula:	C30H50O
SMILES:	CC1CCC2(C)CCC3(C)C(=CCC4C5(C)CCC(O)C(C)(C)C5CCC43C)C2C1C
Mol. weight [g/mol]:	426.72
CAS:	638-95-9

Physical Properties

Property code	Value	Unit	Source
gf	230.57	kJ/mol	Joback Method
hf	-493.41	kJ/mol	Joback Method
hfus	29.29	kJ/mol	Joback Method
hvap	93.17	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	8.025		Crippen Method
mcvol	380.830	ml/mol	McGowan Method
pc	1018.78	kPa	Joback Method
rinpol	3376.00		NIST Webbook
tb	1018.89	K	Joback Method
tc	1259.59	K	Joback Method
tf	661.08	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1563.32	J/mol×K	1018.89	Joback Method

cpg	1617.79	J/mol×K	1059.01	Joback Method
cpg	1677.12	J/mol×K	1099.12	Joback Method
cpg	1742.05	J/mol×K	1139.24	Joback Method
cpg	1813.33	J/mol×K	1179.36	Joback Method
cpg	1891.73	J/mol×K	1219.48	Joback Method
cpg	1977.98	J/mol×K	1259.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C638959&Units=SI

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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