

«beta»-Amyrin

Other names:	Olean-12-en-3-ol, (3«beta»)- Olean-12-en-3«beta»-ol «beta»-Amyrenol «beta»-Amirine Olean-12-en-3-ol
Inchi:	InChI=1S/C30H50O/c1-25(2)15-16-27(5)17-18-29(7)20(21(27)19-25)9-10-23-28(6)13-12
InchiKey:	JFSHUTJDVKUMTJ-UHFFFAOYSA-N
Formula:	C30H50O
SMILES:	CC1(C)CCC2(C)CCC3(C)C(=CCC4C5(C)CCC(O)C(C)(C)C5CCC43C)C2C1
Mol. weight [g/mol]:	426.72
CAS:	559-70-6

Physical Properties

Property code	Value	Unit	Source
gf	232.79	kJ/mol	Joback Method
hf	-457.83	kJ/mol	Joback Method
hfus	21.92	kJ/mol	Joback Method
hvap	92.32	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	8.169		Crippen Method
mcvol	380.830	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	3337.00		NIST Webbook
tb	1023.80	K	Joback Method
tc	1268.67	K	Joback Method
tf	689.22	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1573.52	J/mol×K	1023.80	Joback Method
cpg	1635.98	J/mol×K	1064.61	Joback Method
cpg	1705.07	J/mol×K	1105.42	Joback Method

cpg	1781.73	J/mol×K	1146.24	Joback Method
cpg	1866.89	J/mol×K	1187.05	Joback Method
cpg	1961.46	J/mol×K	1227.86	Joback Method
cpg	2066.37	J/mol×K	1268.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C559706&Units=SI
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

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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