

«beta»-Amyrone

Inchi:	InChI=1S/C30H48O/c1-25(2)15-16-27(5)17-18-29(7)20(21(27)19-25)9-10-23-28(6)13-12
InchiKey:	LIIFBMGUDSHTOU-UHFFFAOYSA-N
Formula:	C30H48O
SMILES:	CC1(C)CCC2(C)CCC3(C)C(=CCC4C5(C)CCC(=O)C(C)(C)C5CCC43C)C2C1
Mol. weight [g/mol]:	424.70
CAS:	638-97-1

Physical Properties

Property code	Value	Unit	Source
gf	254.73	kJ/mol	Joback Method
hf	-422.96	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	8.377		Crippen Method
mcvol	376.530	ml/mol	McGowan Method
pc	1054.83	kPa	Joback Method
rinpol	3327.50		NIST Webbook
tb	1004.11	K	Joback Method
tc	1267.56	K	Joback Method
tf	700.86	K	Joback Method
vc	1.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1519.20	J/mol×K	1004.11	Joback Method
cpg	1582.44	J/mol×K	1048.02	Joback Method
cpg	1652.62	J/mol×K	1091.93	Joback Method
cpg	1730.86	J/mol×K	1135.84	Joback Method
cpg	1818.26	J/mol×K	1179.75	Joback Method
cpg	1915.92	J/mol×K	1223.65	Joback Method
cpg	2024.95	J/mol×K	1267.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638971&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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