

«alpha»-Amyrone

Inchi:	InChI=1S/C30H48O/c1-19-11-14-27(5)17-18-29(7)21(25(27)20(19)2)9-10-23-28(6)15-13
InchiKey:	DIFWJFSELKWGA-UHFFFAOYSA-N
Formula:	C30H48O
SMILES:	CC1CCC2(C)CCC3(C)C(=CCC4C5(C)CCC(=O)C(C)(C)C5CCC43C)C2C1C
Mol. weight [g/mol]:	424.70
CAS:	638-96-0

Physical Properties

Property code	Value	Unit	Source
gf	252.51	kJ/mol	Joback Method
hf	-458.54	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	81.04	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	8.233		Crippen Method
mvol	376.530	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
rinpol	3372.90		NIST Webbook
tb	999.20	K	Joback Method
tc	1256.45	K	Joback Method
tf	672.72	K	Joback Method
vc	1.423	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.94	J/mol×K	999.20	Joback Method
cpg	1567.02	J/mol×K	1042.08	Joback Method
cpg	1626.99	J/mol×K	1084.95	Joback Method
cpg	1692.74	J/mol×K	1127.83	Joback Method
cpg	1765.12	J/mol×K	1170.70	Joback Method
cpg	1845.03	J/mol×K	1213.58	Joback Method
cpg	1933.33	J/mol×K	1256.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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