«beta»-Amyrin acetate

Other names: «beta»-Amyrin (12-oleanenol) acetate
Inchi: InChI=1S/C32H52O2/c1-21(33)34-26-13-14-30(7)24(28(26,4)5)12-15-32(9)25(30)11-10-
InchiKey: UMRPOGLIBDXFNK-CFBPMWJOSA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC2(C)C(CCC3(C)C2CC=C2C4CC(C)(C)CCC4(C)CCC23C)C1(C)C
Mol. weight [g/mol]: 468.75
CAS: 1616-93-9

Physical Properties

Property code	Value	Unit	Source
gf	152.53	kJ/mol	Joback Method
hf	-591.68	kJ/mol	Joback Method
hfus	25.80	kJ/mol	Joback Method
hvap	89.25	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.740		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	922.18	kPa	Joback Method
rinpol	3339.00		NIST Webbook
rinpol	3339.00		NIST Webbook
rinpol	3437.70		NIST Webbook
rinpol	3437.70		NIST Webbook
tb	1053.67	K	Joback Method
tc	1307.40	K	Joback Method
tf	723.10	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1711.32	J/mol×K	1053.67	Joback Method
cpg	1781.21	J/mol×K	1095.96	Joback Method
cpg	1858.58	J/mol×K	1138.25	Joback Method
cpg	1944.46	J/mol×K	1180.54	Joback Method

cpg	2039.84	J/mol×K	1222.82	Joback Method
cpg	2145.73	J/mol×K	1265.11	Joback Method
cpg	2263.13	J/mol×K	1307.40	Joback Method

Sources

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=C1616939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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