Isobauerenol (8-bauerenol) acetate

Inchi: InChI=1S/C32H52O2/c1-20-12-15-29(6)18-19-31(8)24-10-11-25-28(4,5)26(34-22(3)33)14
InchiKey: GXGXUGKOSZFXNS-XKRMTFNLSA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC2(C)C3=C(CCC2C1(C)C)C1(C)CCC2(C)CCC(C)C(C)C2C1(C)CC3
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	148.39	kJ/mol	Joback Method
hf	-618.39	kJ/mol	Joback Method
hfus	31.71	kJ/mol	Joback Method
hvap	91.07	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.740		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	889.47	kPa	Joback Method
rinpol	3387.00		NIST Webbook
tb	1058.41	K	Joback Method
tc	1308.83	K	Joback Method
tf	711.72	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1700.06	J/mol×K	1058.41	Joback Method
cpg	1762.02	J/mol×K	1100.15	Joback Method
cpg	1829.75	J/mol×K	1141.88	Joback Method
cpg	1904.08	J/mol×K	1183.62	Joback Method
cpg	1985.83	J/mol×K	1225.36	Joback Method
cpg	2075.84	J/mol×K	1267.09	Joback Method
cpg	2174.92	J/mol×K	1308.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111285&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