22-Dihydrobrassicasterol acetate

Inchi: InChI=1S/C30H50O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31)
InchiKey: JOBAYBRAHVTSSW-NNRQEXCZSA-N
Formula: C30H50O2
SMILES: CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCC(C)C(C)C)CCC32)C1
Mol. weight [g/mol]: 442.72

Physical Properties

Property code	Value	Unit	Source
gf	129.20	kJ/mol	Joback Method
hf	-647.00	kJ/mol	Joback Method
hfus	39.16	kJ/mol	Joback Method
hvap	88.60	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	8.206		Crippen Method
mcvol	393.260	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	3276.00		NIST Webbook
tb	999.69	K	Joback Method
tc	1231.31	K	Joback Method
tf	557.54	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1504.06	J/mol×K	999.69	Joback Method
cpg	1537.82	J/mol×K	1038.29	Joback Method
cpg	1572.22	J/mol×K	1076.90	Joback Method
cpg	1607.63	J/mol×K	1115.50	Joback Method
cpg	1644.38	J/mol×K	1154.10	Joback Method
cpg	1682.84	J/mol×K	1192.71	Joback Method
cpg	1723.35	J/mol×K	1231.31	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=R110064&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