28-Isofucosterol acetate

Inchi: InChI=1S/C31H50O2/c1-8-23(20(2)3)10-9-21(4)27-13-14-28-26-12-11-24-19-25(33-22(5
InchiKey: UKVGAWCNOIELAQ-NYAPKIOYSA-N
Formula: C31H50O2
SMILES: CC=C(CCC(C)C1CCC2C3CC=C4CC(OC(C)=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	211.73	kJ/mol	Joback Method
hf	-554.93	kJ/mol	Joback Method
hfus	44.17	kJ/mol	Joback Method
hvap	91.25	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	8.516		Crippen Method
mcvol	403.050	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	3374.00		NIST Webbook
rinpol	3374.00		NIST Webbook
tb	1027.05	K	Joback Method
tc	1263.32	K	Joback Method
tf	564.77	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.69	J/mol×K	1027.05	Joback Method
cpg	1584.51	J/mol×K	1066.43	Joback Method
cpg	1621.46	J/mol×K	1105.81	Joback Method
cpg	1659.93	J/mol×K	1145.19	Joback Method
cpg	1700.32	J/mol×K	1184.57	Joback Method
cpg	1743.03	J/mol×K	1223.94	Joback Method
cpg	1788.44	J/mol×K	1263.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110613&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

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