4-epi-Dehydroabietinol acetate

Inchi: InChI=1S/C22H32O2/c1-15(2)17-7-9-19-18(13-17)8-10-20-21(4,14-24-16(3)23)11-6-12-2
InchiKey: SNKPCSRNBVWIIG-UHFFFAOYSA-N
Formula: C22H32O2
SMILES: CC(=O)OCC1(C)CCCC2(C)c3ccc(C(C)C)cc3CCC12
Mol. weight [g/mol]: 328.49
CAS: 24462-15-5

Physical Properties

Property code	Value	Unit	Source
gf	69.76	kJ/mol	Joback Method
hf	-390.48	kJ/mol	Joback Method
hfus	25.81	kJ/mol	Joback Method
hvap	74.49	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.383		Crippen Method
mcvol	282.800	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2451.10		NIST Webbook
rinpol	2451.10		NIST Webbook
tb	833.08	K	Joback Method
tc	1063.93	K	Joback Method
tf	518.72	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.37	J/mol×K	833.08	Joback Method
cpg	941.28	J/mol×K	871.55	Joback Method
cpg	965.10	J/mol×K	910.03	Joback Method
cpg	989.13	J/mol×K	948.50	Joback Method
cpg	1013.66	J/mol×K	986.98	Joback Method
cpg	1038.99	J/mol×K	1025.45	Joback Method
cpg	1065.43	J/mol×K	1063.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24462155&Units=SI

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