

psi-Taraxasterol (20-taraxastenol) 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: BWGPCAAUBIQZKQ-ROISWWGESA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC2(C)C(CCC3(C)C2CCC2C4CC(C)(C)C=CC4(C)CCC23C)C1(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	154.45	kJ/mol	Joback Method
hf	-600.55	kJ/mol	Joback Method
hfus	27.26	kJ/mol	Joback Method
hvap	88.28	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mvol	410.580	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	3443.00		NIST Webbook
rinpol	3443.00		NIST Webbook
tb	1044.02	K	Joback Method
tc	1296.76	K	Joback Method
tf	706.34	K	Joback Method
vc	1.548	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1705.97	J/molxK	1044.02	Joback Method
cpg	1773.88	J/molxK	1086.14	Joback Method
cpg	1848.91	J/molxK	1128.27	Joback Method
cpg	1932.05	J/molxK	1170.39	Joback Method
cpg	2024.31	J/molxK	1212.51	Joback Method
cpg	2126.66	J/molxK	1254.64	Joback Method
cpg	2240.12	J/molxK	1296.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R111423&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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