Isoincensole acetate

Inchi: InChI=1S/C21H34O3/c1-16(2)21-13-12-17(3)10-8-6-7-9-11-19(23-18(4)22)20(5,24-21)14
InchiKey: JGYQPJGHMBZUTL-ZUQWZGOFSA-N
Formula: C21H34O3
SMILES: CC(=O)OC1CCC=CCCC(C)=CCC2(C(C)C)CCC1(C)O2
Mol. weight [g/mol]: 334.49

Physical Properties

Property code	Value	Unit	Source
gf	-152.34	kJ/mol	Joback Method
hf	-654.46	kJ/mol	Joback Method
hfus	25.29	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.349		Crippen Method
mcvol	289.740	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
tb	833.70	K	Joback Method
tc	1074.07	K	Joback Method
tf	471.96	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.89	J/mol×K	833.70	Joback Method
cpg	982.94	J/mol×K	873.76	Joback Method
cpg	1008.26	J/mol×K	913.82	Joback Method
cpg	1033.12	J/mol×K	953.89	Joback Method
cpg	1057.76	J/mol×K	993.95	Joback Method
cpg	1082.43	J/mol×K	1034.01	Joback Method
cpg	1107.38	J/mol×K	1074.07	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=R286403&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