Incensole acetate

Inchi: InChI=1S/C21H34O3/c1-15(2)21-11-10-16(3)8-7-9-17(4)14-19(23-18(5)22)20(6,24-21)12
InchiKey: ILTBJIPOZQCQDI-VTMQPUDVSA-N
Formula: C21H34O3
SMILES: CC(=O)OC1CC(C)=CCCC(C)=CCC2(C(C)C)CCC1(C)O2
Mol. weight [g/mol]: 334.49
CAS: 34701-53-6

Physical Properties

Property code	Value	Unit	Source
gf	-149.87	kJ/mol	Joback Method
hf	-659.77	kJ/mol	Joback Method
hfus	27.00	kJ/mol	Joback Method
hvap	76.12	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.349		Crippen Method
mcvol	289.740	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	2122.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	834.41	K	Joback Method
tc	1069.47	K	Joback Method
tf	488.00	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.44	J/mol×K	834.41	Joback Method
cpg	977.75	J/mol×K	873.59	Joback Method
cpg	1002.49	J/mol×K	912.76	Joback Method
cpg	1026.88	J/mol×K	951.94	Joback Method
cpg	1051.15	J/mol×K	991.12	Joback Method
cpg	1075.54	J/mol×K	1030.29	Joback Method

cpg	1100.29	J/mol×K	1069.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34701536&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

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