Isoincensole

Inchi: InChI=1S/C20H34O2/c1-15(2)20-12-11-17(4)8-6-7-16(3)9-10-18(21)19(5,22-20)13-14-20
InchiKey: SSBZLMMXFQMHDP-NFJHNLFSSA-N
Formula: C20H34O2
SMILES: CC1=CCC2(C(C)C)CCC(C)(O2)C(O)CCC(C)=CCC1
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
gf	-73.29	kJ/mol	Joback Method
hf	-552.72	kJ/mol	Joback Method
hfus	23.61	kJ/mol	Joback Method
hvap	81.59	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.168		Crippen Method
mcvol	274.080	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2249.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2249.00		NIST Webbook
tb	831.69	K	Joback Method
tc	1058.41	K	Joback Method
tf	461.87	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.28	J/mol×K	831.69	Joback Method
cpg	937.34	J/mol×K	869.48	Joback Method
cpg	960.90	J/mol×K	907.26	Joback Method
cpg	984.18	J/mol×K	945.05	Joback Method

cpg	1007.41	J/mol×K	982.83	Joback Method
cpg	1030.80	J/mol×K	1020.62	Joback Method
cpg	1054.57	J/mol×K	1058.41	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=U412984&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