Incensole

Inchi: InChI=1S/C19H32O2/c1-14(2)19-10-9-15(3)7-6-8-16(4)13-17(20)18(5,21-19)11-12-19/h8
InchiKey: WISFQNFBBZKQNS-VAJCHKISSA-N
Formula: C20H34O2
SMILES: CC1=CCC2(C(C)C)CCC(C)(O2)C(O)CC(C)=CCC1
Mol. weight [g/mol]: 306.48
CAS: 22419-74-5

Physical Properties

Property code	Value	Unit	Source
gf	-69.61	kJ/mol	Joback Method
hf	-525.92	kJ/mol	Joback Method
hfus	23.12	kJ/mol	Joback Method
hvap	79.19	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.778		Crippen Method
mcvol	259.990	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2184.30		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	804.54	K	Joback Method
tc	1028.60	K	Joback Method
tf	454.12	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.44	J/mol×K	804.54	Joback Method
cpg	870.38	J/mol×K	841.88	Joback Method
cpg	892.82	J/mol×K	879.23	Joback Method
cpg	914.99	J/mol×K	916.57	Joback Method
cpg	937.10	J/mol×K	953.91	Joback Method

cpg	959.37	J/mol×K	991.25	Joback Method
cpg	982.02	J/mol×K	1028.60	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=C22419745&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

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