8-Hydroxysandaracopimaradiene

Inchi: InChI=1S/C20H32O/c1-6-19(4)11-8-15-14(13-19)16(21)12-17-18(2,3)9-7-10-20(15,17)5/h
InchiKey: BNRZBCUNLMPNJG-BKXYZSJASA-N
Formula: C20H32O
SMILES: C=CC1(C)C=C2C(O)CC3C(C)(C)CCCC3(C)C2CC1
Mol. weight [g/mol]: 288.47

Physical Properties

Property code	Value	Unit	Source
gf	171.02	kJ/mol	Joback Method
hf	-264.32	kJ/mol	Joback Method
hfus	19.42	kJ/mol	Joback Method
hvap	73.30	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.112		Crippen Method
mcvol	257.350	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	2090.00		NIST Webbook
tb	778.28	K	Joback Method
tc	999.91	K	Joback Method
tf	482.70	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.16	J/mol×K	778.28	Joback Method
cpg	868.33	J/mol×K	815.22	Joback Method
cpg	892.53	J/mol×K	852.16	Joback Method
cpg	917.14	J/mol×K	889.09	Joback Method
cpg	942.51	J/mol×K	926.03	Joback Method
cpg	969.00	J/mol×K	962.97	Joback Method
cpg	996.97	J/mol×K	999.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202945&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