Sandaracopimaridiene

Inchi: InChI=1S/C20H32/c1-6-19(4)13-10-16-15(14-19)8-9-17-18(2,3)11-7-12-20(16,17)5/h6,14
InchiKey: XDSYKASBVOZOAG-OTGCGEFBSA-N
Formula: C20H32
SMILES: C=CC1(C)C=C2CCC3C(C)(C)CCCC3(C)C2CC1
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	315.55	kJ/mol	Joback Method
hf	-91.75	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	56.93	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	6.142		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	1939.00		NIST Webbook
rinpol	334.40		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	334.40		NIST Webbook
rinpol	1927.00		NIST Webbook
tb	690.77	K	Joback Method
tc	930.20	K	Joback Method
tf	426.12	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.71	J/mol×K	690.77	Joback Method
cpg	789.62	J/mol×K	730.67	Joback Method
cpg	815.66	J/mol×K	770.58	Joback Method
cpg	841.30	J/mol×K	810.48	Joback Method
cpg	867.00	J/mol×K	850.39	Joback Method

cpg	893.21	J/mol×K	890.29	Joback Method
cpg	920.40	J/mol×K	930.20	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=R324104&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