cis-3,14-Clerodadien-13-ol

Inchi: InChI=1S/C20H34O/c1-7-18(4,21)13-14-20(6)16(3)11-12-19(5)15(2)9-8-10-17(19)20/h7,
InchiKey: YBDUXZKWDIUNSG-UHFFFAOYSA-N
Formula: C20H34O
SMILES: C=CC(C)(O)CCC1(C)C(C)CCC2(C)C(C)=CCCC21
Mol. weight [g/mol]: 290.48
CAS: 374925-73-2

Physical Properties

Property code	Value	Unit	Source
gf	138.41	kJ/mol	Joback Method
hf	-334.61	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.502		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2051.40		NIST Webbook
rinpol	2051.40		NIST Webbook
tb	768.47	K	Joback Method
tc	976.99	K	Joback Method
tf	451.04	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.48	J/mol×K	768.47	Joback Method
cpg	880.47	J/mol×K	803.22	Joback Method
cpg	901.99	J/mol×K	837.98	Joback Method
cpg	923.28	J/mol×K	872.73	Joback Method
cpg	944.57	J/mol×K	907.49	Joback Method
cpg	966.09	J/mol×K	942.24	Joback Method
cpg	988.08	J/mol×K	976.99	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=C374925732&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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