8-«alpha»-Methyl-11,12,13-tris-nor-eremophil-1(10

Inchi: InChI=1S/C13H20O/c1-9-7-11-6-4-5-10(2)13(11,3)8-12(9)14/h6,9-10H,4-5,7-8H2,1-3H3/
InchiKey: IUMBBNVGGDEFBX-GBIKHYSHSA-N
Formula: C13H20O
SMILES: CC1CC2=CCCC(C)C2(C)CC1=O
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	16.22	kJ/mol	Joback Method
hf	-287.18	kJ/mol	Joback Method
hfus	12.41	kJ/mol	Joback Method
hvap	48.79	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.348		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	1484.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2006.00		NIST Webbook
tb	594.93	K	Joback Method
tc	833.28	K	Joback Method
tf	359.23	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.49	J/mol×K	594.93	Joback Method
cpg	478.27	J/mol×K	634.66	Joback Method
cpg	498.76	J/mol×K	674.38	Joback Method
cpg	518.10	J/mol×K	714.11	Joback Method
cpg	536.42	J/mol×K	753.83	Joback Method
cpg	553.85	J/mol×K	793.56	Joback Method
cpg	570.53	J/mol×K	833.28	Joback Method

Sources

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=R198871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume