12,13-bis-nor-6(7->8)abeo-Eremophil-1(10)-en-7-o

Inchi: InChI=1S/C13H20O/c1-9-5-4-6-12-7-11(10(2)14)8-13(9,12)3/h6,9,11H,4-5,7-8H2,1-3H3/t
InchiKey: GMEDUWWEDCATDC-PXVZOOEYSA-N
Formula: C13H20O
SMILES: CC(=O)C1CC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	21.99	kJ/mol	Joback Method
hf	-255.90	kJ/mol	Joback Method
hfus	16.60	kJ/mol	Joback Method
hvap	51.11	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.348		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1478.00		NIST Webbook
rinpol	1478.00		NIST Webbook
tb	576.71	K	Joback Method
tc	800.96	K	Joback Method
tf	344.46	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.84	J/mol×K	576.71	Joback Method
cpg	463.80	J/mol×K	614.09	Joback Method
cpg	482.49	J/mol×K	651.46	Joback Method
cpg	500.06	J/mol×K	688.84	Joback Method
cpg	516.67	J/mol×K	726.21	Joback Method
cpg	532.46	J/mol×K	763.59	Joback Method
cpg	547.60	J/mol×K	800.96	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=R198564&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