11,12,13-tris-nor-8,8-Dimethyleudesm-3,5-dien-7-o

Inchi: InChI=1S/C14H20O/c1-10-6-5-7-14(4)9-13(2,3)12(15)8-11(10)14/h6,8H,5,7,9H2,1-4H3/t1
InchiKey: GGWRXCWEYXHJBW-CQSZACIVSA-N
Formula: C14H20O
SMILES: CC1=CCCC2(C)CC(C)(C)C(=O)C=C12
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	47.19	kJ/mol	Joback Method
hf	-225.93	kJ/mol	Joback Method
hfus	8.47	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.658		Crippen Method
mcvol	179.370	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1626.00		NIST Webbook
rinpol	1626.00		NIST Webbook
tb	626.86	K	Joback Method
tc	873.04	K	Joback Method
tf	411.92	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.19	J/mol×K	626.86	Joback Method
cpg	503.30	J/mol×K	667.89	Joback Method
cpg	522.40	J/mol×K	708.92	Joback Method
cpg	540.77	J/mol×K	749.95	Joback Method
cpg	558.69	J/mol×K	790.98	Joback Method
cpg	576.44	J/mol×K	832.01	Joback Method
cpg	594.30	J/mol×K	873.04	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235995&Units=SI

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