11,12,13-tris-nor-8,8-Dimethyleudesm-5-en-7-one

Inchi: InChI=1S/C14H22O/c1-10-6-5-7-14(4)9-13(2,3)12(15)8-11(10)14/h8,10H,5-7,9H2,1-4H3/
InchiKey: FNKVHQVJAQMJDF-IINYFYTJSA-N
Formula: C14H22O
SMILES: CC1CCCC2(C)CC(C)(C)C(=O)C=C12
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	19.15	kJ/mol	Joback Method
hf	-292.58	kJ/mol	Joback Method
hfus	8.70	kJ/mol	Joback Method
hvap	49.86	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1620.00		NIST Webbook
tb	618.05	K	Joback Method
tc	860.99	K	Joback Method
tf	394.40	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.50	J/mol×K	618.05	Joback Method
cpg	528.58	J/mol×K	658.54	Joback Method
cpg	549.48	J/mol×K	699.03	Joback Method
cpg	569.47	J/mol×K	739.52	Joback Method
cpg	588.83	J/mol×K	780.01	Joback Method
cpg	607.81	J/mol×K	820.50	Joback Method
cpg	626.68	J/mol×K	860.99	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=R236007&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