13-nor-trans-Eudesma-4(15),7-dien-11-one

Inchi: InChI=1S/C14H20O/c1-10-5-4-7-14(3)8-6-12(11(2)15)9-13(10)14/h6,13H,1,4-5,7-9H2,2-3
InchiKey: TUDQWZYQYYRFMJ-UONOGXRCSA-N
Formula: C14H20O
SMILES: C=C1CCCC2(C)CC=C(C(C)=O)CC12
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	79.10	kJ/mol	Joback Method
hf	-178.12	kJ/mol	Joback Method
hfus	14.86	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.658		Crippen Method
mcvol	179.370	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2325.00		NIST Webbook
tb	607.69	K	Joback Method
tc	837.36	K	Joback Method
tf	370.13	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.85	J/mol×K	607.69	Joback Method
cpg	493.52	J/mol×K	645.97	Joback Method
cpg	511.96	J/mol×K	684.25	Joback Method
cpg	529.34	J/mol×K	722.52	Joback Method
cpg	545.82	J/mol×K	760.80	Joback Method
cpg	561.56	J/mol×K	799.08	Joback Method

cpg	576.71	J/mol×K	837.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R397825&Units=SI
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

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