

13-nor-Eudesma-4,6-dien-11-one

Other names:	13-nor-Eudesm-4,6-dien-11-one
Inchi:	InChI=1S/C14H20O/c1-10-5-4-7-14(3)8-6-12(11(2)15)9-13(10)14/h9H,4-8H2,1-3H3/t14-
InchiKey:	MHDZZWJRZISHQQ-CQSZACIVSA-N
Formula:	C14H20O
SMILES:	CC(=O)C1=CC2=C(C)CCCC2(C)CC1
Mol. weight [g/mol]:	204.31

Physical Properties

Property code	Value	Unit	Source
gf	44.43	kJ/mol	Joback Method
hf	-207.18	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	55.75	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.802		Crippen Method
mcvol	179.370	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1692.00		NIST Webbook
rinpol	1692.00		NIST Webbook
ripol	2360.00		NIST Webbook
ripol	2360.00		NIST Webbook
tb	622.32	K	Joback Method
tc	854.06	K	Joback Method
tf	386.49	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.83	J/molxK	622.32	Joback Method
cpg	491.48	J/molxK	660.94	Joback Method
cpg	509.03	J/molxK	699.57	Joback Method
cpg	525.63	J/molxK	738.19	Joback Method

cpg	541.45	J/mol×K	776.82	Joback Method
cpg	556.66	J/mol×K	815.44	Joback Method
cpg	571.43	J/mol×K	854.06	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=R198688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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