

13-nor-7,8-Epoxy-trans-eudesm-4(15)-en-11-one

Inchi:	InChI=1S/C14H20O2/c1-9-5-4-6-13(3)8-12-14(16-12,10(2)15)7-11(9)13/h11-12H,1,4-8H
InchiKey:	BCXYPNGIQHAWNZ-DGKWRVCWSA-N
Formula:	C14H20O2
SMILES:	<chem>C=C1CCCC2(C)CC3OC3(C(C)=O)CC12</chem>
Mol. weight [g/mol]:	220.31

Physical Properties

Property code	Value	Unit	Source
gf	44.40	kJ/mol	Joback Method
hf	-276.41	kJ/mol	Joback Method
hfus	19.11	kJ/mol	Joback Method
hvap	55.64	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.869		Crippen Method
mcvol	178.680	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	1653.00		NIST Webbook
rinpol	1653.00		NIST Webbook
tb	624.27	K	Joback Method
tc	857.58	K	Joback Method
tf	428.06	K	Joback Method
vc	0.680	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.47	J/mol×K	624.27	Joback Method
cpg	528.65	J/mol×K	663.16	Joback Method
cpg	546.71	J/mol×K	702.04	Joback Method
cpg	563.97	J/mol×K	740.93	Joback Method
cpg	580.75	J/mol×K	779.81	Joback Method
cpg	597.38	J/mol×K	818.70	Joback Method
cpg	614.17	J/mol×K	857.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R397974&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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