

12-ethoxy-8 «alpha»,12-epoxy-13,14,15,16-tertanorlabdane

Inchi:	InChI=1S/C17H30O2/c1-5-18-15-11-12-13(19-15)7-8-14-16(2,3)9-6-10-17(12,14)4/h12-1
InchiKey:	OBRGPZOBPRRHJQ-UGQLREHASA-N
Formula:	C17H30O2
SMILES:	CCOC1CC2C(CCC3C(C)(C)CCCC23C)O1
Mol. weight [g/mol]:	266.42

Physical Properties

Property code	Value	Unit	Source
gf	0.88	kJ/mol	Joback Method
hf	-495.21	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	57.55	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.381		Crippen Method
mcvol	229.550	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
ripol	2317.00		NIST Webbook
ripol	2353.00		NIST Webbook
ripol	2348.00		NIST Webbook
ripol	2320.00		NIST Webbook
ripol	2317.00		NIST Webbook
tb	661.50	K	Joback Method
tc	885.04	K	Joback Method
tf	404.97	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.36	J/molxK	661.50	Joback Method
cpg	732.74	J/molxK	698.76	Joback Method
cpg	756.90	J/molxK	736.01	Joback Method
cpg	780.10	J/molxK	773.27	Joback Method
cpg	802.60	J/molxK	810.52	Joback Method

cpg	824.64	J/mol×K	847.78	Joback Method
cpg	846.49	J/mol×K	885.04	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=R344019&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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