

6,12:7,11-Di-epoxy-eudesm-4-ene, epimer A

Other names:	6,12;7,11-Diepoxy-eudesm-4-ene (epimer A)
Inchi:	InChI=1S/C15H22O2/c1-10-5-4-6-13(2)7-8-15-12(11(10)13)16-9-14(15,3)17-15/h12H,4-9
InchiKey:	JFQRIENZNRVMS-MXTXEEQBSA-N
Formula:	C15H22O2
SMILES:	CC1=C2C3OCC4(C)OC34CCC2(C)CCC1
Mol. weight [g/mol]:	234.33

Physical Properties

Property code	Value	Unit	Source
gf	116.21	kJ/mol	Joback Method
hf	-257.49	kJ/mol	Joback Method
hfus	20.45	kJ/mol	Joback Method
hvap	56.16	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.213		Crippen Method
mcvol	186.210	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2384.00		NIST Webbook
tb	641.84	K	Joback Method
tc	888.44	K	Joback Method
tf	474.17	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.07	J/molxK	641.84	Joback Method
cpg	573.12	J/molxK	682.94	Joback Method
cpg	592.26	J/molxK	724.04	Joback Method
cpg	611.07	J/molxK	765.14	Joback Method

cpg	630.08	J/mol×K	806.24	Joback Method
cpg	649.87	J/mol×K	847.34	Joback Method
cpg	670.97	J/mol×K	888.44	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=R198331&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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