(-)-5,11-epoxy-4 «alpha»,5 «beta»,10 «alpha»-eudesm-1-ene

Inchi: InChI=1S/C15H24O/c1-11-6-5-8-14(4)9-7-12-10-15(11,14)16-13(12,2)3/h5,8,11-12H,6-7

InchiKey: ZYBUFGLEPYWGTL-HAOUFUCWSA-N

Formula: C15H24O

SMILES: CC1CC=CC2(C)CCC3CC12OC3(C)C

Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	133.32	kJ/mol	Joback Method
hf	-222.19	kJ/mol	Joback Method
hfus	15.16	kJ/mol	Joback Method
hvap	49.97	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
ripol	1916.00		NIST Webbook
ripol	1916.00		NIST Webbook
tb	593.12	K	Joback Method
tc	832.40	K	Joback Method
tf	392.62	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.37	J/mol×K	593.12	Joback Method
cpg	561.44	J/mol×K	633.00	Joback Method
cpg	582.99	J/mol×K	672.88	Joback Method
cpg	603.47	J/mol×K	712.76	Joback Method
cpg	623.35	J/mol×K	752.64	Joback Method
cpg	643.09	J/mol×K	792.52	Joback Method
cpg	663.14	J/mol×K	832.40	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=R342895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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