(+)-(4S,5R,6S,7R,10S)-6,11-Epoxyeudesmane

Inchi: InChI=1S/C15H26O/c1-10-5-4-7-15(3)8-6-12-11(2)9-16-14(12)13(10)15/h10-14H,4-9H2,
InchiKey: ZDNLXXMBLHEOIY-ZOYAPEJNSA-N
Formula: C15H26O
SMILES: CC1COC2C1CCC1(C)CCCC(C)C21
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	94.53	kJ/mol	Joback Method
hf	-336.95	kJ/mol	Joback Method
hfus	25.51	kJ/mol	Joback Method
hvap	51.84	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.874		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	1534.00		NIST Webbook
tb	593.08	K	Joback Method
tc	819.56	K	Joback Method
tf	336.30	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.60	J/mol×K	593.08	Joback Method
cpg	591.60	J/mol×K	630.83	Joback Method
cpg	615.94	J/mol×K	668.57	Joback Method
cpg	638.82	J/mol×K	706.32	Joback Method
cpg	660.40	J/mol×K	744.06	Joback Method
cpg	680.87	J/mol×K	781.81	Joback Method
cpg	700.40	J/mol×K	819.56	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=R561358&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume