

(+)-6,7-epoxyeudesm-3-ene

Inchi:	InChI=1S/C15H24O/c1-10(2)15-9-8-14(4)7-5-6-11(3)12(14)13(15)16-15/h6,10,12-13H,5,
InchiKey:	PRQISQJIVNJQOR-CVSAEHQPSA-N
Formula:	C15H24O
SMILES:	CC1=CCCC2(C)CCC3(C(C)C)OC3C12
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	146.55	kJ/mol	Joback Method
hf	-227.68	kJ/mol	Joback Method
hfus	18.57	kJ/mol	Joback Method
hvap	51.53	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinsol	1787.00		NIST Webbook
tb	597.82	K	Joback Method
tc	825.69	K	Joback Method
tf	374.00	K	Joback Method
vc	0.727	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.11	J/mol×K	597.82	Joback Method
cpg	559.84	J/mol×K	635.80	Joback Method
cpg	580.19	J/mol×K	673.78	Joback Method
cpg	599.46	J/mol×K	711.75	Joback Method
cpg	617.97	J/mol×K	749.73	Joback Method
cpg	636.02	J/mol×K	787.71	Joback Method
cpg	653.93	J/mol×K	825.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R510484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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

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