

6,12-Epoxy-spiroax-4-ene

Inchi:	InChI=1S/C15H24O/c1-10-6-7-15(8-10)12(3)4-5-13-11(2)9-16-14(13)15/h8,11-14H,4-7,9
InchiKey:	HEQABJJODXEQEX-ANLGBYQQSA-N
Formula:	C15H24O
SMILES:	CC1=CC2(CC1)C(C)CCC1C(C)COC12
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	122.57	kJ/mol	Joback Method
hf	-270.30	kJ/mol	Joback Method
hfus	25.27	kJ/mol	Joback Method
hvap	53.11	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.794		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1577.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1577.00		NIST Webbook
tb	601.89	K	Joback Method
tc	831.52	K	Joback Method
tf	353.82	K	Joback Method
vc	0.718	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.86	J/molxK	601.89	Joback Method
cpg	568.88	J/molxK	640.16	Joback Method
cpg	591.37	J/molxK	678.43	Joback Method
cpg	612.50	J/molxK	716.71	Joback Method
cpg	632.48	J/molxK	754.98	Joback Method
cpg	651.49	J/molxK	793.25	Joback Method
cpg	669.71	J/molxK	831.52	Joback Method

Sources

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=R198797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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