

5,11-Epoxycaadin-1(10)-ene

Inchi:	InChI=1S/C15H24O/c1-9-6-8-12-13-11(9)7-5-10(2)14(13)16-15(12,3)4/h10-14H,1,5-8H2
InchiKey:	QIBQOCDVTFISGY-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	C=C1CCC2C3C1CCC(C)C3OC2(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	159.71	kJ/mol	Joback Method
hf	-246.55	kJ/mol	Joback Method
hfus	26.45	kJ/mol	Joback Method
hvap	51.83	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.792		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1575.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1575.00		NIST Webbook
ripol	1948.00		NIST Webbook
ripol	1941.00		NIST Webbook
tb	587.97	K	Joback Method
tc	808.71	K	Joback Method
tf	353.50	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.98	J/molxK	587.97	Joback Method
cpg	565.68	J/molxK	624.76	Joback Method
cpg	587.92	J/molxK	661.55	Joback Method
cpg	608.86	J/molxK	698.34	Joback Method
cpg	628.66	J/molxK	735.13	Joback Method

cpg	647.50	J/mol×K	771.92	Joback Method
cpg	665.53	J/mol×K	808.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R228581&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
hvac:	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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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