

(+)-«beta»-Costol

Inchi:	InChI=1S/C15H24O/c1-11-5-4-7-15(3)8-6-13(9-14(11)15)12(2)10-16/h13-14,16H,1-2,4-1
InchiKey:	FKWGZOFNSIESOX-ZNMIVQPWSA-N
Formula:	C15H24O
SMILES:	<chem>C=C(CO)C1CCC2(C)CCCC(=C)C2C1</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	130.87	kJ/mol	Joback Method
hf	-189.42	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook
tb	656.63	K	Joback Method
tc	863.91	K	Joback Method
tf	359.05	K	Joback Method
vc	0.740	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.31	J/mol×K	656.63	Joback Method
cpg	590.40	J/mol×K	691.18	Joback Method
cpg	608.49	J/mol×K	725.72	Joback Method
cpg	625.71	J/mol×K	760.27	Joback Method
cpg	642.19	J/mol×K	794.82	Joback Method
cpg	658.05	J/mol×K	829.36	Joback Method
cpg	673.43	J/mol×K	863.91	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=R336697&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
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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