

«beta»-Costol

Inchi:
InchiKey:
Formula:
SMILES:
Mol. weight [g/mol]:
CAS:

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
FKWGZOFNSIESOX-UHFFFAOYSA-N
C15H24O
C=C(CO)C1CCC2(C)CCCC(=C)C2C1
220.35
515-20-8

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	1781.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1774.20		NIST Webbook
rinpol	1756.00		NIST Webbook
ripol	2606.00		NIST Webbook
ripol	2606.00		NIST Webbook
tb	656.63	K	Joback Method
tc	863.91	K	Joback Method
tf	359.05	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C515208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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