«alpha»-Costol

Inchi: InChI=1S/C15H24O/c1-11-5-4-7-15(3)8-6-13(9-14(11)15)12(2)10-16/h5,13-14,16H,2,4,6-
InchiKey: MTJCJJFCDOSALI-ZNMIVQPWSA-N
Formula: C15H24O
SMILES: C=C(CO)C1CCC2(C)CCC=C(C)C2C1
Mol. weight [g/mol]: 220.35
CAS: 65018-15-7

Physical Properties

Property code	Value	Unit	Source
gf	98.12	kJ/mol	Joback Method
hf	-227.35	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	65.08	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1778.40		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1785.00		NIST Webbook
ripol	2604.00		NIST Webbook
ripol	2604.00		NIST Webbook
tb	661.61	K	Joback Method
tc	869.92	K	Joback Method
tf	358.65	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.16	J/mol×K	661.61	Joback Method
cpg	591.06	J/mol×K	696.33	Joback Method
cpg	608.99	J/mol×K	731.05	Joback Method
cpg	626.07	J/mol×K	765.76	Joback Method

cpg	642.44	J/mol×K	800.48	Joback Method
cpg	658.24	J/mol×K	835.20	Joback Method
cpg	673.58	J/mol×K	869.92	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=C65018157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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