«alpha»-Nootkatol

Inchi: InChI=1S/C15H24O/c1-10(2)12-5-6-13-8-14(16)7-11(3)15(13,4)9-12/h8,11-12,14,16H,1,5

InchiKey: GFNWRKNVTHDNPV-NQRDHLDYSA-N

Formula: C15H24O

SMILES: C=C(C)C1CCC2=CC(O)CC(C)C2(C)C1

Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	90.41	kJ/mol	Joback Method
hf	-247.69	kJ/mol	Joback Method
hfus	20.65	kJ/mol	Joback Method
hvap	64.77	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1710.00		NIST Webbook
tb	656.94	K	Joback Method
tc	865.19	K	Joback Method
tf	354.41	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.99	J/mol×K	656.94	Joback Method
cpg	593.37	J/mol×K	691.65	Joback Method
cpg	611.74	J/mol×K	726.36	Joback Method
cpg	629.25	J/mol×K	761.06	Joback Method
cpg	646.00	J/mol×K	795.77	Joback Method
cpg	662.12	J/mol×K	830.48	Joback Method
cpg	677.75	J/mol×K	865.19	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=R506108&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume