7-epi-Nootcatane

Other names: 7-epi-Nootkatane
Inchi: InChI=1S/C15H28/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h11-14H,5-10H2,1-4H3/t
InchiKey: AJWBFJHTFGRNDG-MCBWDKPDSA-N
Formula: C15H28
SMILES: CC(C)C1CCC2CCCC(C)C2(C)C1
Mol. weight [g/mol]: 208.38

Physical Properties

Property code	Value	Unit	Source
gf	125.17	kJ/mol	Joback Method
hf	-262.69	kJ/mol	Joback Method
hfus	14.80	kJ/mol	Joback Method
hvap	47.34	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.885		Crippen Method
mcvol	200.490	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	1519.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1519.00		NIST Webbook
tb	563.62	K	Joback Method
tc	781.30	K	Joback Method
tf	281.03	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.93	J/mol×K	563.62	Joback Method
cpg	566.03	J/mol×K	599.90	Joback Method
cpg	590.56	J/mol×K	636.18	Joback Method
cpg	613.67	J/mol×K	672.46	Joback Method
cpg	635.49	J/mol×K	708.74	Joback Method
cpg	656.17	J/mol×K	745.02	Joback Method

cpg	675.83	J/mol×K	781.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R134179&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
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
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