

Neoisolongifolane, hydroxy-

Other names:	Isolongifolan-7-«alpha»-ol
Inchi:	InChI=1S/C15H26O/c-12(2)7-5-8-15(16)13(3,4)11-6-9-14(12,15)10-11/h11,16H,5-10H2
InchiKey:	CCMWYZQSEJEA EY-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	CC1(C)CCCC2(O)C(C)(C)C3CCC12C3
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	59.27	kJ/mol	Joback Method
hf	-278.80	kJ/mol	Joback Method
hfus	5.85	kJ/mol	Joback Method
hvap	60.52	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.754		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1621.00		NIST Webbook
tb	655.16	K	Joback Method
tc	876.31	K	Joback Method
tf	453.53	K	Joback Method
vc	0.740	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.59	J/mol×K	655.16	Joback Method
cpg	610.07	J/mol×K	692.02	Joback Method
cpg	629.03	J/mol×K	728.88	Joback Method
cpg	647.94	J/mol×K	765.73	Joback Method
cpg	667.27	J/mol×K	802.59	Joback Method
cpg	687.47	J/mol×K	839.45	Joback Method
cpg	709.02	J/mol×K	876.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U159379&Units=SI

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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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