

Alloisolongifolene alcohol

Inchi:	InChI=1S/C15H24O/c1-11(9-16)15-7-4-6-14(3)12(15)5-8-13(14,2)10-15/h12,16H,1,4-10H
InchiKey:	FQJRQKXSGHUMRO-HXSCFSKGSA-N
Formula:	C15H24O
SMILES:	C=C(CO)C12CCCC3(C)C1CCC3(C)C2
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	163.86	kJ/mol	Joback Method
hf	-151.90	kJ/mol	Joback Method
hfus	10.59	kJ/mol	Joback Method
hvap	61.22	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.531		Crippen Method
mvol	191.200	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	651.88	K	Joback Method
tc	866.24	K	Joback Method
tf	421.67	K	Joback Method
vc	0.733	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.64	J/mol×K	651.88	Joback Method
cpg	584.54	J/mol×K	687.61	Joback Method
cpg	601.77	J/mol×K	723.33	Joback Method
cpg	618.71	J/mol×K	759.06	Joback Method
cpg	635.70	J/mol×K	794.78	Joback Method
cpg	653.12	J/mol×K	830.51	Joback Method
cpg	671.33	J/mol×K	866.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R336771&Units=SI
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

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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