

«alpha»-Bisabolen-12-ol

Inchi:	InChI=1S/C15H24O/c1-12-7-9-15(10-8-12)14(3)6-4-5-13(2)11-16/h5-7,15-16H,4,8-11H2
InchiKey:	CUXGFNUZZPYJNJ-LSMSNJBFS-A-N
Formula:	C15H24O
SMILES:	CC(=CCC=C(C)C1CC=C(C)CC1)CO
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	126.72	kJ/mol	Joback Method
hf	-189.67	kJ/mol	Joback Method
hfus	29.15	kJ/mol	Joback Method
hvap	67.12	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.008		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1762.00		NIST Webbook
tb	666.55	K	Joback Method
tc	864.71	K	Joback Method
tf	302.21	K	Joback Method
vc	0.775	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.04	J/mol×K	666.55	Joback Method
cpg	582.17	J/mol×K	699.58	Joback Method
cpg	598.34	J/mol×K	732.60	Joback Method
cpg	613.60	J/mol×K	765.63	Joback Method
cpg	628.02	J/mol×K	798.65	Joback Method
cpg	641.64	J/mol×K	831.68	Joback Method
cpg	654.53	J/mol×K	864.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R442232&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

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

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