

(-)-4 «alpha»-hydroxydihydroagarofuran

Inchi:	InChI=1S/C15H26O2/c1-12(2)11-6-9-13(3)7-5-8-14(4,16)15(13,10-11)17-12/h11,16H,5-1
InchiKey:	XEAXSPJWIVZRTF-FAAHXZRKSA-N
Formula:	C15H26O2
SMILES:	CC1(C)OC23CC1CCC2(C)CCCC3(C)O
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-38.95	kJ/mol	Joback Method
hf	-416.96	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	65.21	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.275		Crippen Method
mvol	201.370	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
ripol	2248.00		NIST Webbook
ripol	2248.00		NIST Webbook
tb	686.38	K	Joback Method
tc	911.90	K	Joback Method
tf	476.58	K	Joback Method
vc	0.752	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.61	J/mol×K	686.38	Joback Method
cpg	646.55	J/mol×K	723.97	Joback Method
cpg	666.31	J/mol×K	761.55	Joback Method
cpg	686.36	J/mol×K	799.14	Joback Method
cpg	707.20	J/mol×K	836.72	Joback Method
cpg	729.29	J/mol×K	874.31	Joback Method
cpg	753.13	J/mol×K	911.90	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=R342880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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