

Dihydro-cis-«alpha»-copaene-8-ol

Inchi:	InChI=1S/C15H26O/c1-8(2)12-11(16)7-15(4)10-6-5-9(3)14(15)13(10)12/h8-14,16H,5-7H
InchiKey:	QULDBKHTWZIUJN-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	CC(C)C1C(O)CC2(C)C3CCC(C)C2C13
Mol. weight [g/mol]:	222.37
CAS:	58569-27-0

Physical Properties

Property code	Value	Unit	Source
gf	69.98	kJ/mol	Joback Method
hf	-364.32	kJ/mol	Joback Method
hfus	25.46	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.322		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
tb	640.39	K	Joback Method
tc	837.41	K	Joback Method
tf	361.87	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.49	J/molxK	640.39	Joback Method
cpg	621.62	J/molxK	673.23	Joback Method
cpg	640.71	J/molxK	706.06	Joback Method
cpg	658.90	J/molxK	738.90	Joback Method
cpg	676.33	J/molxK	771.73	Joback Method
cpg	693.13	J/molxK	804.57	Joback Method
cpg	709.42	J/molxK	837.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58569270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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