1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1ar-(1a«alpha»,4a«alpha»,7«beta»,7a«beta»,7b«a

Other names:	(1aR,4aR,7S,7aR,7bR)-1,1,7-Trimethyl-4-methylenedecahydro-1H-cyclopropa[e]azulen-7
	Spathulenol
	1,1,7-Trimethyl-4-methylenedecahydro-1H-cyclopropa[e]azulen-7-ol-, (1aR-(1a«alpha»,4a«alpha»,7«beta»,7a«beta»,7b«alpha»))-
	(+)-Spathulenol
	Espatulenol
	Spatulenol
Inchi:	InChI=1S/C15H24O/c1-9-5-6-11-13(14(11,2)3)12-10(9)7-8-15(12,4)16/h10-13,16H,1,5-8
InchiKey:	FRMCCTDTYSRUBE-OUZJWQAESA-N
Formula:	C15H24O
SMILES:	C=C1CCC2C(C3C1CCC3(C)O)C2(C)C
Mol. weight [g/mol]:	220.35
CAS:	6750-60-3

Physical Properties

Property code	Value	Unit	Source
gf	115.62	kJ/mol	Joback Method
hf	-245.38	kJ/mol	Joback Method
hfus	18.36	kJ/mol	Joback Method
hvap	62.68	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
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tc	856.86	K	Joback Method
tf	415.17	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.53	J/mol×K	649.17	Joback Method
cpg	594.60	J/mol×K	683.79	Joback Method
cpg	612.82	J/mol×K	718.40	Joback Method
cpg	630.40	J/mol×K	753.02	Joback Method
cpg	647.59	J/mol×K	787.63	Joback Method
cpg	664.58	J/mol×K	822.25	Joback Method
cpg	681.62	J/mol×K	856.86	Joback Method

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

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