(-)-Spathulenol

Other names:	(1aS,4aS,7R,7aS,7bS)-1,1,7-Trimethyl-4-methylenedecahydro-1H-cyclopropa[e]azulen-7
	1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1aS-(1a«alpha»,4a«alpha»,7«beta»)]
	Ent-Spathulenol
	(-)-ent-Spathulenol
	1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, *1aS-(1a«alpha»,4a«alpha»,7«beta»
	«beta»-Spathulenol
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-MLNWTNLKSA-N
Formula:	C15H24O
SMILES:	C=C1CCC2C(C3C1CCC3(C)O)C2(C)C
Mol. weight [g/mol]:	220.35
CAS:	77171-55-2

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
rinpol	1576.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1578.00		NIST Webbook
tb	649.17	K	Joback Method
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

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77171552&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume