Spiro[furan-3(2H),2'-[2H]inden]-2-one, decahydro-3'a,4'-dimethyl-4-methylene-, [2'R-(2'«alpha»,3'a«alpha»,4'«alpha»,7'a«alpha»)]-

Other names:	Spiro[furan-3(2H),2'-indan]-2-one, 3',3'a,4',5',6',7',7'a«beta»-octahydro-3'a«beta»,4'«beta»-dimethyl-4-methylene-, (2'R)-
	Bakkenolid A
	Bakkenolide A
	Fukinanolid
	Fukinanolide
Inchi:	InChI=1S/C15H22O2/c1-10-5-4-6-12-7-15(9-14(10,12)3)11(2)8-17-13(15)16/h10,12H,2,4
InchiKey:	OVXAYHNZXBOVPV-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	C=C1COC(=O)C12CC1CCCC(C)C1(C)C2
Mol. weight [g/mol]:	234.33
CAS:	19906-72-0

Physical Properties

Property code	Value	Unit	Source
gf	34.95	kJ/mol	Joback Method
hf	-334.49	kJ/mol	Joback Method
hfus	15.42	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.322		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
ripol	2549.00		NIST Webbook
ripol	2549.00		NIST Webbook
tb	669.64	K	Joback Method
tc	919.61	K	Joback Method
tf	450.58	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.10	J/mol×K	669.64	Joback Method
cpg	601.69	J/mol×K	711.30	Joback Method

cpg	623.23	J/mol×K	752.96	Joback Method
cpg	644.06	J/mol×K	794.62	Joback Method
cpg	664.52	J/mol×K	836.28	Joback Method
cpg	684.93	J/mol×K	877.95	Joback Method
cpg	705.62	J/mol×K	919.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19906720&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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