Lanciniata furanone F

Other names: (2S,2'S,5R,5'S)-2,5'-Dimethyl-5-(prop-1-en-2-yl)-5'-vinylhexahydro-[2,2'-bifuran]-3(2H)-on
Inchi: InChI=1S/C15H22O3/c1-6-14(4)8-7-13(18-14)15(5)12(16)9-11(17-15)10(2)3/h6,11,13H,1
InchiKey: LQWFUFMRXNEVLA-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: C=CC1(C)CCC(C2(C)OC(C(=C)C)CC2=O)O1
Mol. weight [g/mol]: 250.33
CAS: 148709-42-6

Physical Properties

Property code	Value	Unit	Source
gf	-5.58	kJ/mol	Joback Method
hf	-402.80	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	58.59	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.803		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1536.00		NIST Webbook
tb	679.26	K	Joback Method
tc	921.44	K	Joback Method
tf	423.81	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.67	J/mol×K	679.26	Joback Method
cpg	628.38	J/mol×K	719.62	Joback Method
cpg	649.17	J/mol×K	759.99	Joback Method
cpg	669.31	J/mol×K	800.35	Joback Method
cpg	689.07	J/mol×K	840.72	Joback Method
cpg	708.72	J/mol×K	881.08	Joback Method
cpg	728.55	J/mol×K	921.44	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C148709426&Units=SI

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