

Laciniata furanone H

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:	<chem>C=CC1(C)CCC(C2(C)OC(C=C)C)CC2=O)O1</chem>
Mol. weight [g/mol]:	250.33
CAS:	147663-93-2

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	1553.90		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
tb	679.26	K	Joback Method
tc	921.44	K	Joback Method
tf	423.81	K	Joback Method
vc	0.763	m ³ /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:	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=C147663932&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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