Laciniatafuranone A

Inchi: InChI=1S/C14H20O3/c1-5-14(4)7-6-11(17-14)13-10(15)8-12(16-13)9(2)3/h5,11-13H,1-2,
InchiKey: JFVWSTQFYSQOMC-ZXCYLUJYSA-N
Formula: C14H20O3
SMILES: C=CC1(C)CCC(C2OC(C(=C)C)CC2=O)O1
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
gf	-8.51	kJ/mol	Joback Method
hf	-397.40	kJ/mol	Joback Method
hfus	27.33	kJ/mol	Joback Method
hvap	57.51	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.413		Crippen Method
mcvol	191.110	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	1526.00		NIST Webbook
tb	656.14	K	Joback Method
tc	894.30	K	Joback Method
tf	388.64	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.91	J/mol×K	656.14	Joback Method
cpg	577.19	J/mol×K	695.83	Joback Method
cpg	597.23	J/mol×K	735.53	Joback Method
cpg	616.18	J/mol×K	775.22	Joback Method
cpg	634.17	J/mol×K	814.91	Joback Method
cpg	651.36	J/mol×K	854.61	Joback Method
cpg	667.88	J/mol×K	894.30	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=R226758&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