Ligustilide

Inchi: InChI=1S/C12H12O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h4-8H,2-3H2,1H3/b11-8-
InchiKey: WMBOCUXXNSOQHM-FLIBITNWSA-N
Formula: C12H12O2
SMILES: CCCC=C1OC(=O)c2ccccc21
Mol. weight [g/mol]: 188.22

Physical Properties

Property code	Value	Unit	Source
gf	58.15	kJ/mol	Joback Method
hf	-166.48	kJ/mol	Joback Method
hfus	25.36	kJ/mol	Joback Method
hvap	55.01	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.998		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	618.44	K	Joback Method
tc	853.60	K	Joback Method
tf	391.27	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.95	J/mol×K	618.44	Joback Method
cpg	384.23	J/mol×K	657.63	Joback Method
cpg	397.57	J/mol×K	696.83	Joback Method
cpg	410.03	J/mol×K	736.02	Joback Method
cpg	421.65	J/mol×K	775.21	Joback Method
cpg	432.48	J/mol×K	814.40	Joback Method
cpg	442.57	J/mol×K	853.60	Joback Method

Sources

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=R628887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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