(E)-Ligustilide

Other names: trans-ligustilide
Ligustilide, (E)-
Inchi: InChI=1S/C12H14O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h5,7-8H,2-4,6H2,1H3/b11-
InchiKey: IQVQXVFMNOFTMU-DHZHZOJOSA-N
Formula: C12H14O2
SMILES: CCCC=C1OC(=O)C2=C1CCC=C2
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	28.19	kJ/mol	Joback Method
hf	-224.26	kJ/mol	Joback Method
hfus	24.14	kJ/mol	Joback Method
hvap	54.72	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.874		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1754.00		NIST Webbook
tb	619.28	K	Joback Method
tc	852.20	K	Joback Method
tf	390.51	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.29	J/mol×K	619.28	Joback Method

cpg	406.76	J/mol×K	658.10	Joback Method
cpg	421.25	J/mol×K	696.92	Joback Method
cpg	434.80	J/mol×K	735.74	Joback Method
cpg	447.47	J/mol×K	774.56	Joback Method
cpg	459.30	J/mol×K	813.38	Joback Method
cpg	470.33	J/mol×K	852.20	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=R87786&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume