(Z)-3-Pentylidene-4,5-dihydroisobenzofuran-1(3H)

Inchi: InChI=1S/C13H16O2/c1-2-3-4-9-12-10-7-5-6-8-11(10)13(14)15-12/h6,8-9H,2-5,7H2,1H3
InchiKey: HMAYXYFQOZZPEZ-XFXZXTDPSA-N
Formula: C13H16O2
SMILES: CCCCC=C1OC(=O)C2=C1CCC=C2
Mol. weight [g/mol]: 204.26
CAS: 116964-00-2

Physical Properties

Property code	Value	Unit	Source
gf	36.61	kJ/mol	Joback Method
hf	-244.90	kJ/mol	Joback Method
hfus	26.73	kJ/mol	Joback Method
hvap	56.94	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.264		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1851.30		NIST Webbook
rinpol	1851.30		NIST Webbook
tb	642.16	K	Joback Method
tc	870.52	K	Joback Method
tf	401.78	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.34	J/mol×K	642.16	Joback Method
cpg	457.42	J/mol×K	680.22	Joback Method
cpg	472.49	J/mol×K	718.28	Joback Method
cpg	486.61	J/mol×K	756.34	Joback Method
cpg	499.81	J/mol×K	794.40	Joback Method
cpg	512.16	J/mol×K	832.46	Joback Method
cpg	523.69	J/mol×K	870.52	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=C116964002&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