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

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-FLIBITNWSA-N
Formula: C12H14O2
SMILES: CCCC=C1OC(=O)C2=C1CCC=C2
Mol. weight [g/mol]: 190.24
CAS: 81944-09-4

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	1740.20		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

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=C81944094&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