n-butylidene dihydrophthalide

Inchi: InChI=1S/C12H14O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h4-10H,2-3H2,1H3/b11-8-
InchiKey: XTVWTNWDUGUSNF-FLIBITNWSA-N
Formula: C12H14O2
SMILES: CCCC=C1OC(=O)C2C=CC=CC12
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	32.03	kJ/mol	Joback Method
hf	-242.00	kJ/mol	Joback Method
hfus	27.06	kJ/mol	Joback Method
hvap	52.78	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.586		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
ripol	2676.00		NIST Webbook
tb	599.98	K	Joback Method
tc	831.06	K	Joback Method
tf	356.99	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.28	J/mol×K	599.98	Joback Method
cpg	413.28	J/mol×K	638.49	Joback Method
cpg	429.18	J/mol×K	677.01	Joback Method
cpg	444.03	J/mol×K	715.52	Joback Method
cpg	457.86	J/mol×K	754.04	Joback Method
cpg	470.73	J/mol×K	792.55	Joback Method
cpg	482.68	J/mol×K	831.06	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=R339527&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume