3-Butylidenephthalide, (Z)-

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
CAS: 72917-31-8

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	1684.40		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1678.00		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

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=C72917318&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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