Isobutylidene phthalide

Inchi: InChI=1S/C12H12O2/c1-8(2)7-11-9-5-3-4-6-10(9)12(13)14-11/h3-8H,1-2H3/b11-7-
InchiKey: LYSNVWBBICAAMS-XFFZJAGNSA-N
Formula: C12H12O2
SMILES: CC(C)C=C1OC(=O)c2ccccc21
Mol. weight [g/mol]: 188.22

Physical Properties

Property code	Value	Unit	Source
gf	55.71	kJ/mol	Joback Method
hf	-171.76	kJ/mol	Joback Method
hfus	21.84	kJ/mol	Joback Method
hvap	54.62	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.854		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
ripol	2543.00		NIST Webbook
ripol	2563.00		NIST Webbook
tb	618.00	K	Joback Method
tc	858.31	K	Joback Method
tf	376.27	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.42	J/mol×K	618.00	Joback Method
cpg	385.06	J/mol×K	658.05	Joback Method
cpg	398.71	J/mol×K	698.10	Joback Method
cpg	411.42	J/mol×K	738.15	Joback Method
cpg	423.25	J/mol×K	778.20	Joback Method
cpg	434.25	J/mol×K	818.25	Joback Method
cpg	444.46	J/mol×K	858.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R339512&Units=SI
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

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