3-Butylisobenzofuran-1(3H)-one

Other names: butylphthalide
1(3H)-Isobenzofuranone, 3-butyl-
3-Butylphthalide
Phthalide, 3-butyl-
3-n-Butylphthalide
Inchi: InChI=1S/C12H14O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h4-7,11H,2-3,8H2,1H3
InchiKey: HJXMNVQARNZTEE-UHFFFAOYSA-N
Formula: C12H14O2
SMILES: CCCCC1OC(=O)c2ccccc21
Mol. weight [g/mol]: 190.24
CAS: 6066-49-5

Physical Properties

Property code	Value	Unit	Source
gf	4.98	kJ/mol	Joback Method
hf	-262.85	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.088		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1658.00		NIST Webbook
ripol	2557.00		NIST Webbook
ripol	2585.00		NIST Webbook
tb	607.13	K	Joback Method
tc	835.27	K	Joback Method
tf	376.67	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.74	J/mol×K	607.13	Joback Method

cpg	409.66	J/mol×K	645.15	Joback Method
cpg	424.59	J/mol×K	683.18	Joback Method
cpg	438.56	J/mol×K	721.20	Joback Method
cpg	451.61	J/mol×K	759.22	Joback Method
cpg	463.77	J/mol×K	797.25	Joback Method
cpg	475.10	J/mol×K	835.27	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=C6066495&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume