3-(2-Propynyloxy)-2-benzofuran-1(3h)-one

Inchi: InChI=1S/C11H8O3/c1-2-7-13-11-9-6-4-3-5-8(9)10(12)14-11/h1,3-6,11H,7H2
InchiKey: IUSUHIUAFDBTHY-UHFFFAOYSA-N
Formula: C11H8O3
SMILES: C#CCOC1OC(=O)c2ccccc21
Mol. weight [g/mol]: 188.18
CAS: 61133-38-8

Physical Properties

Property code	Value	Unit	Source
gf	114.63	kJ/mol	Joback Method
hf	-82.53	kJ/mol	Joback Method
hfus	27.68	kJ/mol	Joback Method
hvap	53.96	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	1.505		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	596.79	K	Joback Method
tc	843.27	K	Joback Method
tf	434.60	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.05	J/mol×K	596.79	Joback Method
cpg	342.47	J/mol×K	637.87	Joback Method
cpg	354.99	J/mol×K	678.95	Joback Method
cpg	366.62	J/mol×K	720.03	Joback Method
cpg	377.40	J/mol×K	761.11	Joback Method
cpg	387.35	J/mol×K	802.19	Joback Method
cpg	396.50	J/mol×K	843.27	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=C61133388&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume