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

Inchi: InChI=1S/C11H10O3/c1-2-7-13-11-9-6-4-3-5-8(9)10(12)14-11/h2-6,11H,1,7H2
InchiKey: VUHVYYOSDKVVEP-UHFFFAOYSA-N
Formula: C11H10O3
SMILES: C=CCOC1OC(=O)c2ccccc21
Mol. weight [g/mol]: 190.20
CAS: 61133-37-7

Physical Properties

Property code	Value	Unit	Source
gf	-20.60	kJ/mol	Joback Method
hf	-249.00	kJ/mol	Joback Method
hfus	23.43	kJ/mol	Joback Method
hvap	53.43	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.058		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	603.35	K	Joback Method
tc	837.74	K	Joback Method
tf	385.87	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.04	J/mol×K	603.35	Joback Method
cpg	363.21	J/mol×K	642.42	Joback Method
cpg	376.48	J/mol×K	681.48	Joback Method
cpg	388.87	J/mol×K	720.55	Joback Method
cpg	400.39	J/mol×K	759.61	Joback Method
cpg	411.08	J/mol×K	798.68	Joback Method
cpg	420.94	J/mol×K	837.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61133377&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

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