Benzofuran- 2(3h)-one, 3-allyl-3-phenyl-

Inchi: InChI=1S/C17H14O2/c1-2-12-17(13-8-4-3-5-9-13)14-10-6-7-11-15(14)19-16(17)18/h2-11
InchiKey: DRYGRMOBXKVKNO-UHFFFAOYSA-N
Formula: C17H14O2
SMILES: C=CCC1(c2ccccc2)C(=O)Oc2ccccc21
Mol. weight [g/mol]: 250.29
CAS: 116465-79-3

Physical Properties

Property code	Value	Unit	Source
gf	241.84	kJ/mol	Joback Method
hf	11.15	kJ/mol	Joback Method
hfus	25.53	kJ/mol	Joback Method
hvap	65.50	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.468		Crippen Method
mcvol	195.150	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	745.13	K	Joback Method
tc	1009.34	K	Joback Method
tf	481.58	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.06	J/mol×K	745.13	Joback Method
cpg	558.98	J/mol×K	789.16	Joback Method
cpg	575.10	J/mol×K	833.20	Joback Method
cpg	590.69	J/mol×K	877.23	Joback Method
cpg	605.99	J/mol×K	921.27	Joback Method
cpg	621.28	J/mol×K	965.30	Joback Method
cpg	636.82	J/mol×K	1009.34	Joback Method

Sources

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=C116465793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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