2(3H)-benzofuranone,3-ethoxy-3-phenyl-

Inchi: InChI=1S/C16H14O3/c1-2-18-16(12-8-4-3-5-9-12)13-10-6-7-11-14(13)19-15(16)17/h3-11
InchiKey: DOHHPBAKMKBODF-UHFFFAOYSA-N
Formula: C16H14O3
SMILES: CCOC1(c2ccccc2)C(=O)Oc2ccccc21
Mol. weight [g/mol]: 254.28
CAS: 62231-08-7

Physical Properties

Property code	Value	Unit	Source
gf	40.58	kJ/mol	Joback Method
hf	-225.86	kJ/mol	Joback Method
hfus	25.40	kJ/mol	Joback Method
hvap	66.35	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.886		Crippen Method
mcvol	191.230	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	747.99	K	Joback Method
tc	1008.14	K	Joback Method
tf	494.30	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.39	J/mol×K	747.99	Joback Method
cpg	556.09	J/mol×K	791.35	Joback Method
cpg	571.99	J/mol×K	834.71	Joback Method
cpg	587.29	J/mol×K	878.07	Joback Method
cpg	602.20	J/mol×K	921.42	Joback Method
cpg	616.93	J/mol×K	964.78	Joback Method
cpg	631.69	J/mol×K	1008.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62231087&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume