3-Benzofurancarboxamide, 2,3-dihydro-3-phenyl-

Inchi: InChI=1S/C15H13NO2/c16-14(17)15(11-6-2-1-3-7-11)10-18-13-9-5-4-8-12(13)15/h1-9H,

InchiKey: HVAWGLXOKPVJDA-UHFFFAOYSA-N

Formula: C15H13NO2

SMILES: NC(=O)C1(c2ccccc2)COc2ccccc21

Mol. weight [g/mol]: 239.27

CAS: 92552-62-0

Physical Properties

Property code	Value	Unit	Source
gf	197.28	kJ/mol	Joback Method
hf	-14.09	kJ/mol	Joback Method
hfus	28.91	kJ/mol	Joback Method
hvap	74.86	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	1.850		Crippen Method
mcvol	181.250	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	761.27	K	Joback Method
tc	1030.57	K	Joback Method
tf	525.77	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.26	J/mol×K	761.27	Joback Method
cpg	523.08	J/mol×K	806.15	Joback Method
cpg	537.34	J/mol×K	851.04	Joback Method
cpg	551.35	J/mol×K	895.92	Joback Method
cpg	565.45	J/mol×K	940.81	Joback Method
cpg	579.93	J/mol×K	985.69	Joback Method
cpg	595.12	J/mol×K	1030.57	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=C92552620&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