2-[(3-Oxo-1,3-dihydro-2-benzofuran-1-yl)amino]be
acid

Inchi: InChI=1S/C15H11NO4/c17-14(18)11-7-3-4-8-12(11)16-13-9-5-1-2-6-10(9)15(19)20-13/h1

InchiKey: VAWIUWGDQXKJEU-UHFFFAOYSA-N

Formula: C15H11NO4

SMILES: O=C(O)c1ccccc1NC1OC(=O)c2ccccc21

Mol. weight [g/mol]: 269.25

CAS: 42974-40-3

Physical Properties

Property code	Value	Unit	Source
gf	-43.33	kJ/mol	Joback Method
hf	-311.05	kJ/mol	Joback Method
hfus	38.32	kJ/mol	Joback Method
hvap	93.39	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.666		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	903.65	K	Joback Method
tc	1145.77	K	Joback Method
tf	612.83	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.14	J/mol×K	903.65	Joback Method
cpg	580.97	J/mol×K	944.00	Joback Method
cpg	589.84	J/mol×K	984.36	Joback Method
cpg	597.80	J/mol×K	1024.71	Joback Method
cpg	604.92	J/mol×K	1065.06	Joback Method
cpg	611.25	J/mol×K	1105.42	Joback Method
cpg	616.86	J/mol×K	1145.77	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=C42974403&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