3-Hydroxy-6-nitro-2-benzofuran-1(3h)-one

Inchi: InChI=1S/C8H5NO5/c10-7-5-2-1-4(9(12)13)3-6(5)8(11)14-7/h1-3,7,10H
InchiKey: WUQPXBMPKNIUCE-UHFFFAOYSA-N
Formula: C8H5NO5
SMILES: O=C1OC(O)c2ccc([N+](=O)[O-])cc21
Mol. weight [g/mol]: 195.13
CAS: 77619-93-3

Physical Properties

Property code	Value	Unit	Source
gf	-139.60	kJ/mol	Joback Method
hf	-354.75	kJ/mol	Joback Method
hfus	30.81	kJ/mol	Joback Method
hvap	78.94	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	0.756		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
pc	4924.59	kPa	Joback Method
tb	764.61	K	Joback Method
tc	1011.53	K	Joback Method
tf	548.54	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.63	J/mol×K	764.61	Joback Method
cpg	340.13	J/mol×K	805.76	Joback Method
cpg	347.89	J/mol×K	846.92	Joback Method
cpg	354.94	J/mol×K	888.07	Joback Method
cpg	361.30	J/mol×K	929.22	Joback Method
cpg	367.02	J/mol×K	970.38	Joback Method
cpg	372.10	J/mol×K	1011.53	Joback Method

Sources

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=C77619933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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