6-nitro-3H-2-benzofuran-1-one

Inchi: InChI=1S/C8H5NO4/c10-8-7-3-6(9(11)12)2-1-5(7)4-13-8/h1-3H,4H2
InchiKey: RNWGZXAHUPFXLL-UHFFFAOYSA-N
Formula: C8H5NO4
SMILES: O=C1OCc2ccc([N+](=O)[O-])cc21
Mol. weight [g/mol]: 179.13

Physical Properties

Property code	Value	Unit	Source
gf	4.93	kJ/mol	Joback Method
hf	-182.18	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	62.57	kJ/mol	Joback Method
log10ws	-2.65		Aqueous Solubility Prediction Method
logp	1.265		Crippen Method
mcvol	113.820	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
tb	677.10	K	Joback Method
tc	950.43	K	Joback Method
tf	491.96	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.92	J/mol×K	677.10	Joback Method
cpg	299.42	J/mol×K	722.66	Joback Method
cpg	309.00	J/mol×K	768.21	Joback Method
cpg	317.72	J/mol×K	813.77	Joback Method
cpg	325.63	J/mol×K	859.32	Joback Method
cpg	332.76	J/mol×K	904.88	Joback Method
cpg	339.18	J/mol×K	950.43	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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