Benzofuran, 7-(2,4-dinitrophenoxy)-3-ethoxy-2,3-dihydro-2,2-di

Inchi: InChI=1S/C18H18N2O7/c1-4-25-17-12-6-5-7-15(16(12)27-18(17,2)3)26-14-9-8-11(19(21

InchiKey: NQDMYVDQNBMUIS-UHFFFAOYSA-N

Formula: C18H18N2O7

SMILES: CCOC1c2cccc(Oc3ccc([N+](=O)[O-])cc3[N+](=O)[O-])c2OC1(C)C

Mol. weight [g/mol]: 374.34

CAS: 62059-46-5

Physical Properties

Property code	Value	Unit	Source
gf	109.51	kJ/mol	Joback Method
hf	-337.93	kJ/mol	Joback Method
hfus	54.89	kJ/mol	Joback Method
hvap	103.83	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	4.544		Crippen Method
mcvol	258.550	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
tb	1062.30	K	Joback Method
tc	1332.11	K	Joback Method
tf	791.39	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.50	J/mol×K	1062.30	Joback Method
cpg	884.77	J/mol×K	1107.27	Joback Method
cpg	903.48	J/mol×K	1152.24	Joback Method
cpg	922.88	J/mol×K	1197.20	Joback Method
cpg	943.21	J/mol×K	1242.17	Joback Method
cpg	964.71	J/mol×K	1287.14	Joback Method
cpg	987.63	J/mol×K	1332.11	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=C62059465&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