Benzoic acid, 4'-nitro-4-biphenyl ester

Inchi: InChI=1S/C19H13NO4/c21-19(16-4-2-1-3-5-16)24-18-12-8-15(9-13-18)14-6-10-17(11-7-
InchiKey: XNKFHWLFAVBPKN-UHFFFAOYSA-N
Formula: C19H13NO4
SMILES: O=C(Oc1ccc(-c2ccc([N+](=O)[O-])cc2)cc1)c1ccccc1
Mol. weight [g/mol]: 319.31
CAS: 3916-45-8

Physical Properties

Property code	Value	Unit	Source
gf	228.70	kJ/mol	Joback Method
hf	-4.40	kJ/mol	Joback Method
hfus	40.46	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	4.481		Crippen Method
mcvol	232.150	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
tb	952.25	K	Joback Method
tc	1229.64	K	Joback Method
tf	623.96	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.48	J/mol×K	952.25	Joback Method
cpg	691.32	J/mol×K	998.48	Joback Method
cpg	700.76	J/mol×K	1044.71	Joback Method
cpg	708.92	J/mol×K	1090.95	Joback Method
cpg	715.93	J/mol×K	1137.18	Joback Method
cpg	721.89	J/mol×K	1183.41	Joback Method
cpg	726.92	J/mol×K	1229.64	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=C3916458&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