N-(3-Bromo-4-hydroxy-phenyl)-4-nitro-benzenesu N,O-dimethyl-

Inchi: InChI=1S/C14H13BrN2O5S/c1-16(11-5-8-14(22-2)13(15)9-11)23(20,21)12-6-3-10(4-7-12
InchiKey: IMQVVLNPUMHDNI-UHFFFAOYSA-N
Formula: C14H13BrN2O5S
SMILES: COc1ccc(N(C)S(=O)(=O)c2ccc([N+](=O)[O-])cc2)cc1Br
Mol. weight [g/mol]: 401.23

Physical Properties

Property code	Value	Unit	Source
gf	-149.96	kJ/mol	Joback Method
hf	-396.11	kJ/mol	Joback Method
hfus	51.16	kJ/mol	Joback Method
hvap	99.41	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.191		Crippen Method
mcvol	239.460	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	2891.00		NIST Webbook
rinpol	2891.00		NIST Webbook
tb	888.66	K	Joback Method
tc	1140.63	K	Joback Method
tf	634.61	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.32	J/mol×K	888.66	Joback Method
cpg	662.57	J/mol×K	930.66	Joback Method
cpg	671.44	J/mol×K	972.65	Joback Method
cpg	678.97	J/mol×K	1014.65	Joback Method
cpg	685.21	J/mol×K	1056.64	Joback Method
cpg	690.22	J/mol×K	1098.64	Joback Method
cpg	694.03	J/mol×K	1140.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374408&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume